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THREE-DIMENSIONAL STRUCTURES AND MODELS OF FC RECEPTORS AND USES THEREOF

Abstract:

Abstract of WO9940117

Disclosed are crystals, crystal structure Fc gamma Rlla protein, three-dimensional coordinates of Fc gamma Rlla protein, and structures and models derived from the Fc gamma Rlla structure. Also disclosed are crystals of Fc epsilon Rl protein and three-dimensional coordinates of Fc epsilon Rl protein monomers and dimers derived from the Fc gamma Rlla structure. Also disclosed are three-dimensional coordinates of Fc gamma Rlllb proteins and models of Fc gamma Rlllb derived from the Fc gamma Rlla structure. The present invention also includes methods to produce such crystals, crystal structures and models. Uses of such crystals, crystal structures and models are also disclosed, including structure based drug design and therapeutic compositions. Data supplied from the esp@cenet database - Worldwide

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(54) Title: THREE-DIMENSIONAL STRUCTURES AND MODELS OF Fc RECEPTORS AND USES THEREOF

(57) Abstract

Disclosed are crystals, crystal structure $Fc\gamma RIIa$ protein, three-dimensional coordinates of $Fc\gamma RIIa$ protein, and structures and models derived from the $Fc\gamma RIIa$ structure. Also disclosed are crystals of $Fc\epsilon RI$ protein and three-dimensional coordinates of $Fc\epsilon RI$ protein monomers and dimers derived from the $Fc\gamma RIIa$ structure. Also disclosed are three-dimensional coordinates of $Fc\gamma RIIIb$ proteins and models of $Fc\gamma RIIIb$ derived from the $Fc\gamma RIIa$ structure. The present invention also includes methods to produce such crystals, crystal structures and models. Uses of such crystals, crystal structures and models are also disclosed, including structure based drug design and therapeutic compositions.

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THREE DIMENSIONAL STRUCTURES AND MODELS OF FC RECEPTORS AND USES THEREOF

5 FIELD OF THE INVENTION

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The present invention relates to three dimensional structures of Fc receptors (FcR), including crystalline FcqRIIa, crystalline FccRI, three dimensional coordinates of FcqRIIa protein, a three dimensional structure of FcqRIIa, three dimensional structures of FcR, and particularly FccRI and FcqRIIIb, derived from the structure of FcqRIIa, models thereof, and uses of such structures and models.

15 BACKGROUND OF THE INVENTION

Fc receptors (FcR) are a family of highly related receptors that are specific for the Fc portion of immunoglobulin (Ig). These receptors have major roles in normal immunity and resistance to infection and provide the humoral immune system with a cellular effector arm. Receptors have been defined for each of the immunoglobulin classes and as such are defined by the class of Ig of which they bind (i.e. Fc gamma receptor (Fc γ R) bind gamma immunoglobulin (IgG), Fc epsilon receptor (FceR) bind epsilon immunoglobulin (IgE), Fc alpha receptor (Fc α R) bind alpha immunoglobulin (IgA)). Among the FcYR receptors, three subfamily members have been defined; FcyRI, which is a high a affinity receptor for IgG; FcYRII, which are low affinity receptors for IgG that avidly bind to aggregates immune complexes; and FcYRIII, which are low affinity receptors that bind to immune complexes. These receptors are highly related structurally but perform different The structure and function of $Fc\gamma RII$ is of functions. interest because of its interaction with immune complexes and its association with disease.

FcyR are expressed on most hematopoietic cells, and through the binding of IgG play a key role in homeostasis of the immune system and host protection against infection.

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FCYRII is a low affinity receptor for IgG that essentially binds only to IgG immune complexes and is expressed on a variety of cell types including, for example monocytes, macrophages, neutrophils, eosinophils, platelets and B FcyRII is involved in various immune and lymphocytes. inflammatory responses including antibody-dependent cell-mediated cytotoxicity, clearance of immune complexes, release of inflammatory mediators and regulation of antibody production. The binding of IgG to an FcyR can lead to disease indications that involve regulation by FCYR. For example, the autoimmune disease thrombocytopenia purpura involves tissue (platelet) damage resulting from FcyR-dependent IgG immune complex activation of platelets or their destruction by FcYR+ phagocytes. In addition, various inflammatory disease are known to involve IgG immune complexes (e.g. rheumatoid arthritis, systemic lupus erythematosus), including type II and type III hypersensitivity reactions. Type ΙI and type hypersensitivity reactions are mediated by IgG, which can activate either complement-mediated or phagocytic effector mechanisms, leading to tissue damage.

The elucidation of the protein structure of FcyRIIa, indeed any FcR is of importance in formulation of therapeutic and diagnostic reagents for disease management. Until the discovery of the present invention, the structure and resulting mechanism by which FcyRIIa regulates immune responses was unknown. Thus, despite the general multifunctional role of FcyRIIa, development of useful reagents for treatment or diagnosis of disease was hindered by lack of structural information of the receptor. The linear nucleic acid and amino acid sequence of FcyRIIa have been previously reported (Hibbs et al. Proc. Natl. Acad. Sci. USA, vol. 85, pp. 2240-2244, 1988). Mutagenesis studies to identify regions of human FcyRIIa (Hulett et al., Eur. J Immunol. , vol. 23, pp.

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40-645, 1993; Hulett et al., J. Biol. Chem., vol. 69, pp. 15287-15293 1994; and Hulett et al., J. Biol. Chem., vol. 270, pp. 21188-21194, 1995), human FcyRIIIb (Hibbs et al., J. Immunol., vol. 152, p. 4466, 1994; and Tamm et al., J. Biol. Chem. , vol. 271, p. 3659, 1996) and mouse FcyRI (Hulett et al., J. Immunol., vol. 148, pp. 1863-1868, 1991) have defined important regions of IgG binding to the FcYR. Information based on linear sequences, however, cannot accurately predict three dimensional structure of the protein and its functional domains. Huber et al. (J. Mol. Biol., vol. 230, pp. 1077-1083, 1993) have described crystal formation of neonatal rat Fc receptor protein (FcRn). Burmeister et al. (Nature, vol. 372, pp. 336-343, 1994; and Nature, vol. 372, pp. 379-383, 1994) have described the structure of FcRn crystals. FcRn, however, is closely related to major histocompatability protein complex and not related to the leukocyte FcYR family by function or structure. Thus, the protein structure of FcRn is not predictive of the FcR structure of the present invention.

FceR are expressed on mast cells, and through the binding of IgE, trigger an inflammatory immune response which is primarily due to the release of inflammatory mediators upon degranulation of the mast cell (e.g., histamine and serotonin). Release of these mediators causes localized vascular permeability and increase in fluids in the local tissues, including an influx of polymorphonuclear cells into the site. Thus, binding of IgE to an FceRI can lead to disease indications that involve discharge of fluids from the gut and increased mucus secretion and bronchial contraction, such indications typically being associated with diseases involving allergic inflammation. Therefore, the elucidation of protein structure of FceRI is of importance in the formulation of therapeutic and diagnostic reagents for disease management,

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and in particular, for the management of diseases related to allergic inflammation and other Th2-based immune responses. As for the FcYR described above, the linear nucleic acid and amino acid sequences of human FceRI have been previously reported (Kochan et al., 1998, Nuc. Acid. Res. 16:3584). Until the discovery of the present invention, however, the structure and resulting mechanism by which FceR regulates immune responses was unknown. Thus, despite the knowledge of the general action of FceRI, the development of useful reagents for treatment or diagnosis of disease, such as diseases associated with allergic inflammation, was hindered by lack of structural information of the receptor.

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Therefore, there is a need in the art to elucidate the three dimensional structures and models of the Fc receptors, and to use such structures and models in therapeutic strategies, such as drug design.

SUMMARY OF THE INVENTION

The present invention relates to crystalline FcyRIIa and crystalline FceRI, three dimensional coordinates of FcyRIIa protein, the three dimensional structure of FcyRIIa, three dimensional structures and models of Fc receptors (FcR) derived from the structure of FcyRIIa, including FceRI and FcyRIIIb, and uses of such structures and models. Obtaining such crystals is an unexpected result. It is well known in the protein crystallographic art that obtaining crystals of quality sufficient for determining the structure of a protein is unpredictable. In particular, obtaining crystals of quality sufficient for determining the three dimensional (3-D) structure of FcyRIIa has not been achievable until the crystallization of FcyRIIa as disclosed in the present application. such, determination of the three dimensional structure of FcyRIIa has not been possible until the discovery of the

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present invention. Additionally, until the discovery of the present invention, derivation of the three dimensional structure and models of other Fc receptor (FcR) proteins has not been possible. The present inventors are also the first to define the three dimensional structure and provide three dimensional models for drug design for FceRI and FcyRIIIb.

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Accordingly, one object of the present invention is to provide crystals of sufficient quality to obtain a determination of the three dimensional structure of FcyRIIa to high resolution, preferably to the resolution of about 1.8 angstrom. The present invention also includes methods for producing crystalline FcyRIIa.

Yet another object of the present invention is to provide crystals of FceRI protein, preferably of sufficient quality to obtain a determination of the three dimensional structure of FceRI to high resolution. The present invention also includes methods for producing crystalline FCERI.

The value of the crystals of FcγRIIa and Fc∈RI extends 20 beyond merely being able to obtain such crystals. knowledge obtained concerning the FcyRIIa crystal structure, for example, has been used by the present inventors to define the heretofore unknown tertiary structure of the FcyRIIa protein, to model and derive 25 atomic coordinates for the heretofore unknown tertiary structure of the FceRI protein and the heretofore unknown tertiary structure of the FcyRIIIb protein, and can be additionally used to model the heretofore unknown tertiary 30 structure of other FcR proteins having substantially related linear amino acid sequence, such as for other members of the Fc γR protein family and the Fc αRI protein. There are three members of the FcyR family of proteins, FcyRII and FCYRIII, all of which immunoregulatory molecules and all of which bind to IgG.

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Comparison of nucleic acid and amino acid sequences of the $Fc\gamma R$ family of receptors indicates that the receptors are highly homologous. In addition, each member of the $Fc\gamma R$ family of receptors belongs to the Ig super family of molecules, an assignment based on well established criteria (Hulett et al. 1994, ibid.). Moreover, FcyRII, FcyRIII, FceRI and Fc α RI each contain Ig-like domains, indicating the similarity between these receptors. FcyRI contains three Ig-like domains. The first and second domains, however, of FcyRI are substantially homologous to the Ig-like domains of FcyRII, FcyRIII, FceRI and FcoRI. Current methods of tertiary structure determination that do not rely on x-ray diffraction techniques and thus do not require crystallization of the protein (e.g., computer modeling and nuclear magnetic resonance techniques) enable derivation and refinement of models of other FcyR proteins, and $Fc\alpha RI$ protein, extrapolated from a three dimensional structure of FcyRIIa protein. Thus, knowledge of the three dimensional structure of FcyRIIa protein has provided a starting point for investigation into the structure of all of these proteins.

Accordingly, a second object of the present invention is to provide information regarding the structure of FcyRIIa protein and models, atomic coordinates and derived three dimensional structures of other members of the FcyR family of proteins, FceRI and Fc α RI protein.

The knowledge of the three dimensional structure of FcyRIIa and models of other FcR provides a means for designing and producing compounds that regulate immune function and inflammation in an animal, including humans (i.e., structure based drug design). For example, chemical compounds can be designed to block binding of immunoglobulin to an Fc receptor protein using various computer programs and models.

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Another embodiment of the present invention is to provide a three dimensional computer image of the three dimensional structure of an FcR.

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Another embodiment of the present invention is to provide a computer-readable medium encoded with a set of three dimensional coordinates selected from the group of the three dimensional coordinates represented in Table 1, the three dimensional coordinates represented in Table 2, the three dimensional coordinates represented in Table 3, the three dimensional coordinates represented in Table 4, and the three dimensional coordinates represented in Table 5, wherein, using a graphical display software program, the three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

Accordingly, a third object of the present invention is to provide methods for using a three dimensional such as FcyRIIa, and structures, structure of FcR, coordinates and models derived using such structure, for designing reagents for the treatment and diagnosis of disease, such as by binding to or mimicking the action of FcR protein, binding to or mimicking the action of an cellular signal disrupting immunoglobulin (Ig), transduction through an FcR protein by, for example, preventing dimerization of two FcR proteins, or enhancing cellular signal transduction or binding to an FcR by, for example, enhancing dimerization of two FcR proteins.

The knowledge of the three dimensional structure of FcR also provides a means for designing proteins that have altered beneficial functions by analyzing the structure and interactions between individual amino acids of the protein. For example, therapeutic proteins having improved binding to Ig or immune complexes of Ig can be designed to be used as therapeutic compounds to prevent immune complex binding

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to cells or enhance biological responses such as cellular signal transduction upon binding of FcR to Ig or complexes thereof. Thus recombinant soluble FcR engineered to contain improvements can be produced on the basis of the knowledge of the three dimensional structure.

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Accordingly, a fourth object of the present invention is to provide for an extrapolation of the three dimensional structure of FcR to create recombinant protein having altered biological activity.

One embodiment of the present invention is a model of FcR protein, wherein the model represents the three dimensional structure of FcR protein, in which the structure substantially conforms to the atomic coordinates represented by Table 1. Other embodiments of the present invention are the three dimensional structure of an FcyRIIa protein which substantially conforms to the coordinates represented by Table 1; the three dimensional structure of a dimeric FcYRIIa protein which substantially conforms to the atomic coordinates represented by Table 2; the three dimensional structure of a monomeric FceRI protein which substantially conforms the atomic to coordinates represented by Table 3; the three dimensional structure of a dimeric FceRI protein which substantially conforms to the atomic coordinates represented by Table 4; the three dimensional structure of a dimeric FcyRIIIb protein which substantially conforms to the coordinates represented by Table 5 and models representing such structures. Further embodiments of the present invention relate to a set of three dimensional coordinates of an FcyRIIa protein, wherein said coordinates are represented in Table 1; a set of three dimensional coordinates of a dimeric FcyRIIa protein, wherein said coordinates are represented in Table 2; a set of three dimensional coordinates of an FceRI protein, wherein said coordinates are represented in Table 3; a set of three

dimensional coordinates of an FceRI protein, wherein said coordinates are represented in Table 4; and a set of three dimensional coordinates of FcyRIIIb, wherein said coordinates are represented in Table 5. The present invention also includes methods to use such structures including structure based drug design and methods to derive models and images of target FcR structures.

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Another embodiment of the present invention is a composition comprising FcyRIIa protein in a crystalline form. Yet another embodiment of the present invention is a composition comprising FceRI protein in a crystalline form.

Yet another embodiment of the present invention is a method for producing crystals of FcyRIIa, comprising combining FcyRIIa protein with a mother liquor buffer selected from the group consisting of an acetate salt buffer and a sulphate buffer, and inducing crystal formation to produce said FcyRIIa crystals.

The present invention also includes a method for producing crystals of FceRI, comprising combining FceRI protein with a mother liquor buffer selected from the group consisting of an acetate salt buffer, a sodium cacodylate buffer and a sodium citrate buffer, and inducing crystal formation to produce said FceRI crystals.

The present invention also includes a therapeutic composition that, when administered to an animal, reduces IgG-mediated tissue damage, said therapeutic composition comprising an inhibitory compound that inhibits the activity of an FcyRIIa protein, said inhibitory compound being identified by the method comprising: (a) providing a three dimensional structure of an FcyRIIa protein; (b) using said three dimensional structure to design a chemical compound selected from the group consisting of a compound that inhibits binding of FcyRIIa protein to IgG, a compound that substantially mimics the three dimensional structure

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of FcyRIIa protein and a compound that inhibits binding of FcyRIIa protein with a molecule that stimulates cellular signal transduction through an FcyRIIa protein; (c) chemically synthesizing said chemical compound; and (d) evaluating the ability of said synthesized chemical compound to reduce IgG-mediated tissue damage.

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Another embodiment of the present invention is a therapeutic composition that is capable of stimulating an IgG humoral immune response in an animal. Yet another embodiment of the present invention is a therapeutic composition that improves the therapeutic affects of an antibody that is administered to an animal to treat, by opsinization or FcYR-dependent effector functions (e.g. cytotoxicity, FcyR-medicated antibody-dependent cellular mediators), of release phagocytosis or particular disease, including, but not limited to, cancer or infectious disease (e.g. oral infections such as HIV, herpes, bacterial infections, yeast infections or parasite infections). Such a therapeutic composition includes one or more stimulatory compounds that have increased binding to IgG, enhance binding of IgG to FcYR, enhance dimer formation of an FcyR and/or enhance signal transduction through the FcYR. Also included in the present invention is a method to stimulate a humoral immune response. The method includes the step of administering to an animal a therapeutic composition of the present invention.

The present invention also includes a therapeutic composition that, when administered to an animal, reduces IgG-mediated tissue damage, said therapeutic composition comprising an inhibitory compound that inhibits the activity of an FcyRIIIb protein, said inhibitory compound being identified by the method comprising: (a) providing a three dimensional structure of an FcyRIIIb protein; (b) using said three dimensional structure to design a chemical compound selected from the group consisting of a compound

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that inhibits binding of FcyRIIIb protein to IgG, a compound that substantially mimics the three dimensional structure of FcyRIIIb protein and a compound that inhibits binding of FcyRIIIb protein with a molecule that stimulates cellular signal transduction through an FcyRIIIb protein; (c) chemically synthesizing said chemical compound; and (d) evaluating the ability of said synthesized chemical compound to reduce IgG-mediated tissue damage.

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One embodiment of the present invention is therapeutic composition that is capable of reducing IgE-mediated responses. Such therapeutic compositions are capable of reducing IgE-mediated responses resulting from IgE-mediated hypersensitivity, IgE-mediated release of inflammatory modulators or other biological mechanisms involved in IgE-mediated recruitment of inflammatory cells that involves FceR protein. Such a therapeutic composition of the present invention can: (1) inhibit (i.e., prevent, block) binding of FceR protein on a cell having an FceR protein (e.g., mast cells) to an IgE immune complex by interfering with the IgE binding site of an FceR protein; (2) inhibit precipitation of IgE or IgE immune complexes (i.e., prevent Fc:Fc interactions between two IgE); (3) inhibit immunoglobulin-mediated cellular signal transduction by interfering with the binding of an IgE to a cell surface receptor; and (4) inhibit FceR-mediated cellular signal transduction by interfering with the binding of a cell signal inducing molecule (i.e., a molecule that induces cellular signal transduction through an FceR protein) to an FceR protein. Such therapeutic compositions include one or more inhibitory compounds that inhibit binding of IgE to FceR protein, IgE to IgE, IgE to a cell surface receptor, or a cell signal inducing molecule to FceR protein. Also included in the present invention are methods to reduce IgE-mediated responses, such as IgEmediated inflammation.

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Another embodiment of the present invention is a therapeutic composition that is capable of stimulating a IgE humoral immune response in an animal. Yet another embodiment of the present invention is a therapeutic composition that improves the therapeutic affects of an antibody that is administered to an animal to treat, by opsinization or FceR-dependent effector functions (e.g. phagocytosis or release of cellular mediators), particular disease. Such a therapeutic composition includes one or more stimulatory compounds that have increased binding to IgE, enhance binding of IgE to FceRI, enhance dimer formation of FceRI and/or otherwise enhance signal transduction through the FceRI. Also included in the present invention is a method to stimulate a humoral immune response. method The includes the step administering to an animal a therapeutic composition of the present invention.

BRIEF DESCRIPTION OF THE FIGURES

- Fig. 1 is a scanned image of SDS-PAGE analysis of PsFcyRIIa protein during the purification process.
 - Fig. 2 is a scanned image of two-dimensional NEPHGE analysis of purified PsFc γ RIIa protein.
 - Fig. 3 illustrates Langmuir plots of purified PsFcyRIIa protein binding to different isotypes of human immunoglobulin G.
 - Fig. 4 illustrates a graphical representation of the dimer of PFc γ RIIa.
- Fig. 5 illustrates the positions of the beta sheets in FcyRIIa Domains 1 and 2 and compares amino acid sequences of isomorphs of FcyRII.
 - Fig. 6 illustrates the stereo view of the Fc γ RIIa structure shown in Fig. 4.
- Fig. 7 illustrates the location of amino acids involved in binding of FcyRIIa to IgG.

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Fig. 8 illustrates an expanded view of an IgG binding region showing position and side chains of the involved amino acids.

Fig. 9 illustrates an expanded view of an IgG binding region showing amino acids which when mutated to alanine improves IgG binding to $Fc\gamma RIIa$.

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Fig. 10 illustrates an expanded view of the region of one Fc γ RIIa monomer that contributes to the dimer interface.

Fig. 11 illustrates a comparison of the amino acid sequence of FcyRIIa protein with the amino acid sequences of FcyRI, FcyRIIIb and FceRI protein.

Fig. 12 illustrates a comparison of structural features shared by Fc γ RIIa, Fc γ RII and Fc ε RI proteins.

Fig. 13 illustrates a sequence alignment of the amino acid sequences of FcyRIIa and FceRI.

Fig. 14 is a scanned image illustrating a worm representation of the structure of an FceRI monomer.

Fig. 15 is a scanned image illustrating a worm representation of the structure of an FceRI dimer.

Fig. 16 is a scanned image illustrating a molecular surface representation of an FceRI dimer model.

Fig. 17 is a schematic representation of target sites in the FcR structure for drug design.

Fig. 18 illustrates a sequence alignment of the amino acid sequences of FcyRIIa and FcyRIIIb.

DETAILED DESCRIPTION OF THE INVENTION

The present invention relates to the discovery of the three-dimensional structure of Fc receptor (FcR) proteins, models of such three-dimensional structures, a method of structure based drug design using such structures, the compounds identified by such methods and the use of such compounds in therapeutic compositions. More particularly,

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the present invention relates to novel crystals of Fc gamma receptor IIa (FcyRIIa), novel crystals of Fc epsilon receptor I (FceRI), methods of production of such crystals, three dimensional coordinates of FcyRIIa protein, a three dimensional structure of FcyRIIa protein, FcR structures and models derived from the FcyRIIa structure, including FceRI and FcyRIIIb, and uses of such structure and models to derive other FcR structures and in drug design strategies. It is to be noted that the term "a" or "an" entity refers to one or more of that entity; for example, a compound refers to one or more compounds or at least one compound. As such, the terms "a" (or "an"), "one or more" and "at least one" can be used interchangeably herein. is also to noted that the terms be "comprising", "including", and "having" can be used interchangeably. Furthermore, a compound "selected from the group consisting of" refers to one or more of the compounds in the list that follows, including mixtures (i.e., combinations) of two or more of the compounds. According to the present invention, an isolated, or pure, protein, is a protein that has been removed from its natural milieu. As such, "isolated" and "biologically pure" do not necessarily reflect the extent to which the protein has been purified. An isolated protein of the present invention can be obtained from its natural source, can be produced using recombinant DNA technology or can be produced by chemical synthesis. also to be noted that the terms "tertiary" and "three dimensional" can be used interchangeably. It is also to be noted that reference to an "FcR protein" can also be recited simply as "FcR" and such terms can be used to refer to a the complete FcR protein, a portion of the FcR protein, such as a polypeptide, and/or a monomer or a dimer of the FcR protein. When reference is specifically made to a monomer or dimer, for example, such term is typically used in conjunction with the FcR protein name.

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The production of the crystal structure of FcyRIIa has been described in detail in U.S. Provisional Application Serial No. 60/073,972, filed February 6, 1998. The entire disclosure of U.S. Provisional Application Serial No. 60/073,972 is incorporated herein by reference in its entirety.

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One embodiment of the present invention includes a model of an Fc receptor, in which the model represents a three dimensional structure of an Fc receptor (FcR) Another embodiment of the present invention protein. includes the three dimensional structure of an FcR protein. A three dimensional structure of an FcR protein encompassed by the present invention substantially conforms with the atomic coordinates represented in any one of Tables 1-5. According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of an FcR protein which is sufficiently spatially similar to at least a portion of a specified three dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 1) to allow the three dimensional structure of the FcR protein to be modeled or calculated (i.e., by molecular replacement) using the particular set of atomic coordinates as a basis for determining the atomic coordinates defining the three dimensional configuration of the FcR protein. According to the present invention, a three dimensional structure of a dimer of a first FcR can substantially conform to the atomic coordinates which represent a three dimensional structure of a monomer of a second FcR, and vice versa. In the first instance, at least a portion of the structure of the first FcR protein (i.e., a monomer of the first FcR protein dimer) substantially conforms to the atomic coordinates which represent the three dimensional configuration of the second FcR monomer. In the second reversed case, a first monomeric FcR protein substantially

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conforms to at least a portion of the second FcR protein (i.e., a monomer of the second FcR protein dimer). Similarly, a three dimensional structure of a given portion or chain of a first FcR can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second FcR.

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More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 1.5 Å for the backbone atoms in secondary structure elements in each domain, and more preferably, less than about 1.3 Å for the backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, less than about 0.5 Å, and most preferably, less than about 0.3 Å for the backbone atoms in secondary structure elements in each In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such recited average root-mean-square the has structure deviation (RMSD) value, and most preferably, about 100% of such structure has the recited average root-mean-square In an even more preferred deviation (RMSD) value. "substantially of definition above embodiment, the conforms" can be extended to include atoms of amino acid side chains. As used herein, the phrase "common amino acid side chains" refers to amino acid side chains that are common to both the structure which substantially conforms to a given set of atomic coordinates and the structure that actually represented by such atomic coordinates. structure dimensional three а Preferably, substantially conforms to a given set of atomic coordinates

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is a structure wherein at least about 50% of the common amino acid side chains have an average root-mean-square deviation (RMSD) of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, less than about 0.5 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the common amino acid side chains have the recited average root-meansquare deviation (RMSD) value, and more preferably, at least about 90% of the common amino acid side chains have the recited average root-mean-square deviation (RMSD) value, and most preferably, about 100% of the common amino acid side chains have the recited average root-mean-square deviation (RMSD) value.

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A three dimensional structure of an FcR protein which substantially conforms to a specified set of atomic coordinates can be modeled by a suitable modeling computer program such as MODELER (A. Sali and T.L. Blundell, J. Mol. Biol., vol. 234:779-815, 1993 as implemented in the Insight II Homology software package (Insight II (97.0), MSI, San Diego)), using information, for example, derived from the following data: (1) the amino acid sequence of the FcR protein; (2) the amino acid sequence of the related portion(s) of the protein represented by the specified set atomic coordinates having a three dimensional configuration; and, (3) the atomic coordinates of the specified three dimensional configuration. A three dimensional structure of an FcR protein which substantially conforms to a specified set of atomic coordinates can also be calculated by a method such as molecular replacement, which is described in detail below.

A suitable three dimensional structure of an FcR protein for use in modeling or calculating the three

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dimensional structure of another FcR protein comprises the set of atomic coordinates represented in Table 1. The set of three dimensional coordinates set forth in Table 1 is standard Protein Data Bank represented in According to the present invention, an FcR protein selected FcyRIIa, FcyRIIb, from the group of FcyRI, have a three dimensional FceRI and FcaRI FcvRIIIb, structure which substantially conforms to the set of atomic coordinates represented by Table 1. As used herein, a three dimensional structure can also be a most probable, or significant, fit with a set of atomic coordinates. According to the present invention, a most probable or significant fit refers to the fit that a particular FcR protein has with a set of atomic coordinates derived from that particular FcR protein. Such atomic coordinates can be derived, for example, from the crystal structure of the protein such as the coordinates determined for the FcyRIIa structure provided herein, or from a model of the structure of the protein as determined herein for FceRI and FcyRIIIb. For example, the three dimensional structure of a monomeric FcyRIIa protein, including a naturally occurring or recombinantly produced FcyRIIa protein, substantially conforms to and is a most probable fit, or significant fit, with the atomic coordinates of Table 1. The three that FcvRIIa structure of crystal dimensional determined by the present inventors comprises the atomic coordinates of Table 1. Also as an example, the three dimensional structure of an FccRI protein substantially conforms to the atomic coordinates of Table 1 and both substantially conforms to and is a most probable fit with atomic coordinates of Table 3, and the three dimensional structure of the model of FceRI monomer determined by the present inventors comprises the atomic coordinates of Table 3. This definition can be applied to the other FcR proteins in a similar manner.

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A preferred structure of an FcR protein according to the present invention substantially conforms to the atomic coordinates, and the B-values and/or the thermal parameters represented in Table 1. Such values as listed in Table 1 can be interpreted by one of skill in the art. A more preferred three dimensional structure of an FcR protein substantially conforms to the three dimensional coordinates represented in Table 1. An even more preferred three dimensional structure of an FcR protein is a most probable fit with the three dimensional coordinates represented in Table 1. Methods to determine a substantially conforming and probable fit are within the expertise of skill in the art and are described herein in the Examples section.

A preferred FcR protein that has a three dimensional structure which substantially conforms to the atomic coordinates represented by Table 1 includes an FcR protein having an amino acid sequence that is at least about 25%, preferably at least about 30%, more preferably at least about 40%, more preferably at least about 50%, more preferably at least about 60%, more preferably at least about 70%, more preferably at least about 80% and more preferably at least about 90%, identical to an amino acid sequence of an FcyRIIa protein, preferably an amino acid sequence including SEQ ID NO:3, SEQ ID NO:10, SEQ ID NO:11 and/or SEQ ID NO:12, across the full-length of the FcR sequence when using, for example, a sequence alignment program such as the DNAsis™ program (available from Hitachi Software, San Bruno, CA) or the MacVector™ program (available from the Eastman Kodak Company, New Haven, CT) or the GCY™ program (available from "GCY", University of Wisconsin, Madison, WI), such alignment being performed for example, using the standard default values accompanying such alignment programs.

One embodiment of the present invention includes a three dimensional structure of FcyRIIa protein. A suitable

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three dimensional structure of FcyRIIa protein substantially conforms with the atomic coordinates represented in Table 1. A suitable three dimensional structure of FcyRIIa also substantially conforms with the atomic coordinates represented by Tables 2-5. A suitable three dimensional structure of FcyRIIa protein also comprises the set of atomic coordinates represented in The set of three dimensional coordinates of Table 1. FcyRIIa protein is represented in standard Protein Data A preferred structure of FcyRIIa protein Bank format. substantially conforms to the atomic coordinates, and the B-values and/or the thermal parameters represented in Table 1 (monomeric FcyRIIa) or Table 2 (dimeric FcyRIIa). values as listed in Table 1 can be interpreted by one of skill in the art. A more preferred three dimensional structure of FcyRIIa protein has a most probable fit with the three dimensional coordinates represented in Table 1.

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One embodiment of the present invention includes a three dimensional structure of FccRI protein. A suitable three dimensional structure of FceRI protein substantially conforms with the atomic coordinates represented in Table 1, Table 2, Table 3, Table 4 or Table 5. A more suitable three dimensional structure of FceRI protein substantially conforms with the sets of atomic coordinates represented in Table 3 (monomeric FceRI) or Table 4 (dimeric FceRI). suitable three dimensional structure of FceRI protein also comprises the set of atomic coordinates represented in Tables 3 or 4. The sets of three dimensional coordinates of FccRI protein are represented in standard Protein Data Bank Such coordinates as listed in Tables 1-5 can be interpreted by one of skill in the art. A more preferred three dimensional structure of FceRI protein has a probable fit with the three dimensional coordinates represented in Table 3 or Table 4. One embodiment of the present invention includes a three dimensional structure of

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FcyRIIIb protein. A suitable three dimensional structure of FcyRIIIb protein substantially conforms with the atomic coordinates represented in Table 1, Table 2, Table 3, Table 4 or Table 5. An even more suitable three dimensional structure of FcyRIIIb protein substantially conforms with the set of atomic coordinates represented in Table 5. suitable three dimensional structure of FcyRIIIb protein also comprises the set of atomic coordinates represented in Table 5. The sets of three dimensional coordinates of FcyRIIIb protein are represented in standard Protein Data Bank format. A more preferred three dimensional structure of FcyRIIIb protein has a most probable fit with the three dimensional coordinates represented in Table 5. dimensional structure of any FcR protein can be modeled using methods generally known in the art based on information obtained from analysis of an FcvRIIa crystal, and from other FcR structures which are derived from an FcyRIIa crystal. The Examples section below discloses the production of an FcyRIIa crystal, the production of an FccRI crystal, the three dimensional structure of an FcyRIIa protein monomer and dimer derived from the FcyRIIa crystal, and the model of the three dimensional structure of an FccRI protein monomer and dimer using methods generally known in the art based on the information obtained from analysis of an FcyRIIa crystal. It is an embodiment of the present invention that the three dimensional structure of a crystalline FcR, such as the crystalline FcyRIIa, can be used to derive the three dimensional structure of any other FcR, such as the FceRI disclosed herein. Subsequently, the derived three dimensional structure of such an FcR (e.g., FceRI) derived from the crystalline structure of FcyRIIa can be used to derive the three dimensional structure of other FcR, such as FcRyIII. Therefore, the novel discovery herein of the crystalline FcyRIIa and the three dimensional structure of

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FcyRIIa permits one of ordinary skill in the art to now derive the three dimensional structure, and models thereof, of any FcR. The derivation of the structure of any FcR can now be achieved even in the absence of having crystal structure data for such other FcR, and when the crystal structure of another FcR is available, the modeling of the three dimensional structure of the new FcR can be refined using the knowledge already gained from the FcyRIIa It is an advantage of the present invention that, in the absence of crystal structure data for other FcR proteins, the three dimensional structures of other FcR proteins can be modeled, taking into account differences in the amino acid sequence of the other FcR. Indeed, the recent report of the crystallization of the monomeric FceRI and publication of a model of the receptor (Garman et al., December 23, 1998, Cell 95:951-961) subsequent to the priority filing dates of the present application has confirmed that the monomeric FceRI protein determined by the present inventors comprising the atomic coordinates represented in Table 3 has the overall gross structural features of the three dimensional structure of crystalline FceRI reported in Garman et al. Although the atomic coordinates of the crystalline FceRI structure of Garman et al. are not currently publicly available, a review of the structural representations and discussion in indicates that the three dimensional Garman et al. structure of the crystalline FceRI is expected to substantially conform to the atomic coordinates represented by Table 3. Moreover, the novel discoveries of the present invention allow for structure based drug design of compounds which affect the activity of virtually any FcR, and particularly, of FcyR and FceRI.

Crystals are derivatized with heavy atom compounds such as complexes or salts of Pt, Hg, Au and Pb and X-ray diffraction data are measured for native and derivatized

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Differences in diffraction intensities for crystals. native crystals and derivatized crystals can be used to determine phases for these data by the methods of MIR (muliple Isomorphous Replacement) or SIRAS (single isomorphous replacement with anomolous scattering). Fourier transform of these data yield a low resolution electron density map for the protein. This electron density can be modified by image enhancement techniques. A molecular model for the protein is then placed in the electron density. This initial (partial) structure can be refined using a computer program (such as XPLOR) modifying the parameters which describe the structure to minimize the difference between the measured and calculated diffraction patterns, while simultaneously restraining the model to conform to known geometric and chemical properties of proteins. New phases and a thus a new electron density map can be calculated for protein. Using this map as a guide the molecular model of the structure may be improved manually. This procedure is repeated to give the structure of the protein, represented herein for FcyRIIa as a set of atomic coordinates in Table 1.

One embodiment of the present invention includes a three dimensional structure of FcyRIIa protein, in which the atomic coordinates of the FcyRIIa protein are generated by the method comprising: (a) providing FcyRIIa protein in crystalline form; (b) generating an electron-density map of the crystalline FcyRIIa protein; and (c) analyzing the electron-density map to produce the atomic coordinates.

According to the present invention, a three dimensional structure of FcyRIIa protein of the present invention can be used to derive a model of the three dimensional structure of another FcR protein (i.e., a structure to be modeled). As used herein, a "structure" of a protein refers to the components and the manner of arrangement of the components to constitute the protein.

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As used herein, the term "model" refers to a representation in a tangible medium of the three dimensional structure of a protein, polypeptide or peptide. For example, a model can be a representation of the three dimensional structure in an electronic file, on a computer screen, on a piece of paper (i.e., on a two dimensional medium), and/or as a ball-and-stick figure. Physical three-dimensional models are tangible and include, but are not limited to, stick models and space-filling models. The phrase "imaging the model on a computer screen" refers to the ability to express (or represent) and manipulate the model on a computer screen using appropriate computer hardware and software technology known to those skilled in the art. Such technology is available from a variety of sources including, for example, Evans and Sutherland, Salt Lake City, Utah, and Biosym Technologies, San Diego, CA. phrase "providing a picture of the model" refers to the ability to generate a "hard copy" of the model. copies include both motion and still pictures. screen images and pictures of the model can be visualized in а number of formats including space-filling representations, α carbon traces, ribbon diagrams (see, for example, Fig. 14 which is a two dimensional ribbon diagram model of a three-dimensional structure of human FceRI protein) and electron density maps.

Suitable target FcR structures to model using a method of the present invention include any FcR protein, polypeptide or peptide, including monomers, dimers and multimers of an FcR protein, that is substantially structurally related to an FcyRIIa protein. A preferred target FcR structure that is substantially structurally related to an FcyRIIa protein includes a target FcR structure having an amino acid sequence that is at least about 25%, preferably at least about 30%, more preferably at least about 40%,

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more preferably at least about 50%, more preferably at least about 60%, more preferably at least about 70%, more preferably at least about 80% and more preferably at least about 90%, identical to an amino acid sequence of an FcyRIIa protein, preferably an amino acid sequence including SEQ ID NO:3, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, SEQ ID NO:14 and/or SEQ ID NO:15, across the full-length of the target FcR structure sequence when using, for example, a sequence alignment program such as the DNAsis™ program (available from Hitachi Software, San Bruno, CA) or the MacVector™ program (available from the Eastman Kodak Company, New Haven, CT) or the $GC\gamma^{TM}$ program (available from "GCY", University of Wisconsin, Madison, WI), such alignment being performed for example, using the standard default values accompanying such programs. More preferred target FcR structures to model include proteins comprising amino acid sequences that are at least about 50%, preferably at least about 60%, more preferably at least about 70%, more preferably at least about 80%, more preferably at least about 90%, and more preferably at least about 95%, identical to amino acid sequence SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13 when comparing preferred regions of the sequence, such as the amino acid sequence for Domain 1 or Domain 2 of any one of the amino acid sequences, when using a DNA alignment program disclosed herein to align the amino acid sequences. A more preferred target FcR structure to model includes a structure comprising FcYRI, FcYRIIa, FcYRIIb, FcYRIIc, FcYRIIIb, FceRI or FcaRI protein, more preferably a structure comprising the amino acid sequence SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13 and more preferably a structure consisting of the amino

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acid sequence SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13.

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Preferred target FcR structures to model also include, but are not limited to, derivations of Fc receptor proteins, such as an Fc receptor having one or more amino acid residues substituted, deleted or added (referred to herein as Fc receptor mutants), or proteins encoded by natural allelic variants of a nucleic acid molecule encoding an Fc receptor. A preferred Fc receptor protein to model includes FcyRIIayTm (i.e., an FcyRIIa protein from which the transmembrane domain has been deleted), mutants or natural allelic variants of a nucleic acid molecule encoding FcyRI, FCYRIIa, FCYRIIb, FcγRIIIb, FccRI, FcαRI protein. More preferred Fc receptor proteins to model include Fc receptor proteins having an amino acid sequence including SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13 or mutants or natural allelic variants of SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13. According to the present invention, an amino acid sequence for FcyRIIb is represented herein as SEQ ID NO:5, an amino acid sequence for FcyRIIc is represented herein as SEQ ID NO:6, an amino acid sequence for Fc γ RI is represented herein as SEQ ID NO:7, an amino acid sequence for FcyRIII is represented herein as SEQ ID NO:8, an amino acid sequence for FceRI is represented herein as SEQ ID NO:9 and as set forth in Fig. 13, and an amino acid sequence for $Fc\alpha RI$ is represented herein as SEQ ID NO:13. It is noted that the nucleotide and amino acid sequences for all of the above-known FcR are known and publicly available. Preferred allelic variants to model include, but are not limited to, FcyRIIa allelic variants having a glutamine at residue 27 of SEQ ID NO:3

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and an arginine at residue 131 of SEQ ID NO:3, represented herein as SEQ ID NO:10; a tryptophan at residue 27 of SEQ ID NO:3 and a histidine at residue 131 of SEQ ID NO:3, represented herein as SEQ ID NO:11; or a tryptophan at residue 27 of SEQ ID NO:3 and an arginine at residue 131 of SEO ID NO:3, represented herein as SEQ ID NO:12.

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As used herein, a "natural allelic variant" refers to alternative forms of a gene that occupies corresponding loci on homologous chromosomes. Allelic variants typically encode proteins having similar activity to that of the protein encoded by the gene to which they are being compared. Allelic variants can also comprise alterations in the 5' or 3' untranslated regions of the gene (e.g., in regulatory control regions). Allelic variants are well known to those skilled in the art and would be expected to be found within a given group of genes encoding an Fc receptor in a given species of animal.

As used herein, "mutants of a nucleic acid molecule encoding an Fc receptor" refer to nucleic acid molecules modified by nucleotide insertions, deletions and/or Preferably, a mutant of an Fc receptor substitutions. nucleic acid molecule comprises modifications such that the protein encoded by the mutant of an Fc receptor nucleic acid molecule (i.e., an Fc receptor protein mutant) has one or more epitopes that can be targeted by a humoral or cellular immune response against a non-mutated Fc receptor More preferably, the nucleic acid molecule protein. encoding a mutant Fc receptor protein can form a stable hybrid with a nucleic acid sequence encoding a non-mutated nucleic acid molecule under stringent receptor hybridization conditions. Even more preferably, nucleic acid molecule encoding a mutant Fc receptor protein can form a stable hybrid, under stringent hybridization conditions, with a nucleic acid sequence encoding an amino acid sequence including SEQ ID NO:3, SEQ ID NO:5, SEQ ID

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NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13.

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As used herein, stringent hybridization conditions refer to standard hybridization conditions under which nucleic acid molecules are used to identify similar nucleic acid molecules. Such standard conditions are disclosed, for example, in Sambrook et al., Molecular Cloning: A Laboratory Manual, Cold Spring Harbor Labs Press, 1989. Sambrook et al., ibid., is incorporated by reference herein in its entirety (see specifically, pages 9.31-9.62, 11.7 and 11.45-11.61). In addition, formulae to calculate the appropriate hybridization and wash conditions to achieve hybridization permitting varying degrees of mismatch of nucleotides are disclosed, for example, in Meinkoth et al., 1984, Anal. Biochem. 138, 267-284; Meinkoth et al., ibid., is incorporated by reference herein in its entirety.

More particularly, stringent hybridization conditions, as referred to herein, refer to conditions which permit isolation of nucleic acid molecules having at least about 70% nucleic acid sequence identity with the nucleic acid molecule being used to probe in the hybridization reaction, more particularly at least about 75%, and most particularly at least about 80%. Such conditions will vary, depending on whether DNA:RNA or DNA:DNA hybrids are being formed. Calculated melting temperatures for DNA: DNA hybrids are 10°C less than for DNA:RNA hybrids. In particular embodiments, stringent hybridization conditions for DNA: DNA hybrids include hybridization at an ionic strength of 0.1X SSC (0.157 M Na⁺) at a temperature of between about 20°C and about 35°C, more preferably, between about 28°C and about 40°C, and even more preferably, between about 35°C and about 45°C. In particular embodiments, stringent hybridization conditions for DNA:RNA hybrids include hybridization at an ionic strength of 0.1% SSC (0.157 M Na*) at a temperature of between about 30°C and about 45°C, more preferably, between

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about 38°C and about 50°C, and even more preferably, between about 45°C and about 55°C. These values are based on calculations of a melting temperature for molecules larger than about 100 nucleotides, 0% formamide and a G + C content of about 50%. Alternatively, T_m can be calculated empirically as set forth in Sambrook et al., supra, pages 11.55 to 11.57.

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A model of the present invention can be derived using conserved structural features between the known three dimensional structure of one FcR protein, such as FcyRIIa, and another target FcR structure. Such structural features include, but are not limited to, amino acid sequence, conserved di-sulphide bonds, and β -strands or β -sheets that are highly conserved in immunoglobulin superfamily members. For example, Figs. 5, 11 and 12 illustrate the relationship of β -strands with the linear amino acid sequence of various Fc receptor proteins. Preferably, a model of the present invention is derived by starting with the backbone of the three dimensional structure of FcyRIIa protein. Individual residues are then replaced according to the amino acid sequence of the target FcR structure at residues that differ from the amino acid sequence of an FcyRIIa protein. Care is taken that replacement of residues does not disturb the tertiary structure of the backbone. While procedures to model target FcR structures are generally known in the art, the present invention provides the first three dimensional structure of FcyRIIa protein and the first three dimensional structures of protein substantially related to a member of the family of FcyR receptors, an Thus, the present invention FceRI and an FcyRIIIb. provides essential information to produce accurate, and therefore, useful models of a member of the family of FcYR receptors, of the FceRI receptor and of the FcαRI receptor. As discussed above, once the three dimensional structure of a second FcR has been derived from a determined three

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dimensional structure of a first FcR such as FcyRIIa disclosed herein, the second FcR three dimensional structure can be used to derive (i.e., model or calculate) the three dimensional structure of another FcR.

According to the present invention, a structure can be modeled using techniques generally described by, for example, Sali, Current Opinions in Biotechnology, vol. 6, pp. 437-451, 1995, and algorithms can be implemented in program packages such as Homology 95.0 (in the program Insight II, available from Biosym/MSI, San Diego, CA). Use of Homology 95.0 requires an alignment of an amino acid sequence of a known structure having a known three dimensional structure with an amino acid sequence of a target structure to be modeled. The alignment can be a pairwise alignment or a multiple sequence alignment including other related sequences (for example, using the method generally described by Rost, Meth. Enzymol., vol. 266, pp. 525-539, 1996) to improve accuracy. Structurally conserved regions can be identified by comparing related structural features, or by examining the degree of sequence homology between the known structure and the target structure. Certain coordinates for the target structure are assigned using known structures from the known structure. Coordinates for other regions of the target structure can be generated from fragments obtained from known structures such as those found in the Protein Data Bank maintained by Brookhaven National Laboratory, Upton, Conformation of side chains of the target structure NY. can be assigned with reference to what is sterically allowable and using a library of rotamers and their frequency of occurrence (as generally described in Ponder and Richards, J. Mol. Biol., vol. 193, pp. 775-791, 1987). The resulting model of the target structure, can be refined by molecular mechanics (such as embodied in the

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program Discover, available from Biosym/MSI) to ensure that the model is chemically and conformationally reasonable.

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Accordingly, one embodiment of the present invention is a method to derive a model of the three dimensional structure of a target FcR structure, the method comprising the steps of: (a) providing an amino acid sequence of an FcyRIIa protein and an amino acid sequence of a target FcR structure; (b) identifying structurally conserved regions shared between the FcyRIIa amino acid sequence and the target FcR structure amino acid sequence; (c) determining atomic coordinates for the target FcR structure by assigning said structurally conserved regions of the target FcR structure to a three dimensional structure using a three dimensional structure of an FcyRIIa protein based on atomic coordinates that substantially conform to the atomic coordinates represented in Table 1, to derive a model of the three dimensional structure of the target structure A model according to the present amino acid sequence. invention has been previously described herein. Preferably The method can the model comprises a computer model. further comprise the step of electronically simulating the structural assignments to derive a computer model of the three dimensional structure of the target structure amino acid sequence. Suitable target structures to model include polypeptides and peptides of Fc receptors proteins, disclosed herein, including monomers and dimers of such receptors. Preferred amino acid sequences to model are disclosed herein.

Another embodiment of the present invention is a method to derive a computer model of the three dimensional structure of a target FcR structure for which a crystal has been produced (referred to herein as a "crystallized target A suitable method to produce such a model structure"). includes the method comprising molecular replacement. Methods of molecular replacement are generally known by

those of skill in the art (generally described in Brunger, Meth. Enzym., vol. 276, pp. 558-580, 1997; Navaza and Saludjian, Meth. Enzym., vol. 276, pp. 581-594, 1997; Tong and Rossmann, Meth. Enzym., vol. 276, pp. 594-611, 1997; and Bentley, Meth. Enzym., vol. 276, pp. 611-619, 1997, 5 each of which are incorporated by this reference herein in their entirety) and are performed in a software program including, for example, XPLOR. According to the present invention, X-ray diffraction data is collected from the crystal of a crystallized target structure. The X-ray 10 diffraction data is transformed to calculate a Patterson The Patterson function of the crystallized target structure is compared with a Patterson function calculated from a known structure (referred to herein as a 15 search structure). The Patterson function crystallized target structure is rotated on the search structure Patterson function to determine the correct orientation of the crystallized target structure in the The translation function is then calculated to crystal. determine the location of the target structure with respect 20 to the crystal axes. Once the crystallized target structure has been correctly positioned in the unit cell, initial phases for the experimental data can be calculated. These phases are necessary for calculation of an electron density map from which structural differences can be 25 observed and for refinement of the structure. Preferably, the structural features (e.g., amino acid sequence, conserved di-sulphide bonds, and β -strands or β -sheets) of the search molecule are related to the crystallized target structure. Preferably, a crystallized target FcR structure 30 useful in a method of molecular replacement according to the present invention has an amino acid sequence that is at least about 25%, more preferably at least about 30%, more preferably at least about 40%, more preferably at least about 50%, more preferably at least about 60%, more 35

preferably at least about 70%, more preferably at least about 80% and more preferably at least about 90% identical to the amino acid sequence of the search structure (e.g., FcyRIIa), when the two amino acid sequences are compared using a DNA alignment program disclosed herein. Α preferred search structure of the present invention includes an FcyRIIa protein comprising an amino acid sequence including SEQ ID NO:3, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, SEQ ID NO:14 or SEQ ID NO:15. A more preferred search structure of the present invention includes an FcyRIIa protein having a three dimensional structure that substantially conforms with the atomic coordinates listed in Table 1. Preferably, a Patterson function of a crystalline FcyRIIa protein is derived from X-ray diffraction of an FcyRIIa crystal of the present invention. A preferred target FcR structure for use in a molecular replacement strategy of the present invention includes FcyRI, FcyRIIb, FcyRIIc, FcyRIII, FceRI and/or FcαRI, and most preferably, FceRI and FcγRIIIb.

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A preferred embodiment of the present invention includes a method to derive a three dimensional structure of a crystallized target FcR structure (i.e. a crystallized FcR protein), said method comprising the steps of: (a) comparing the Patterson function of a crystallized target FcR structure with the Patterson function of crystalline FcyRIIa protein to produce an electron-density map of said crystallized target FcR structure; and (b) analyzing the electron-density map to produce the three dimensional structure of the crystallized target FcR structure.

Another embodiment of the present invention is a method to determine a three dimensional structure of a target structure, in which the three dimensional structure of the target FcR structure is not known. Such a method is useful for identifying structures that are related to the three dimensional structure of an FcyRIIa protein based

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only on the three dimensional structure of the target structure. Thus, the present method enables identification of structures that do not have high amino acid identity FcyRIIa protein but which do share dimensional structure similarities. A preferred method to determine a three dimensional structure of a target FcR structure comprises: (a) providing an amino acid sequence of a target structure, wherein the three dimensional structure of the target structure is not known; (b) analyzing the pattern of folding of the amino acid sequence in a three dimensional conformation by fold recognition; and (c) comparing the pattern of folding of the target structure amino acid sequence with the three dimensional structure of FcyRIIa protein to determine the three dimensional structure of the target structure, wherein the of the FcvRIIa protein structure dimensional coordinates atomic substantially conforms to the Preferred methods of fold represented in Table 1. recognition include the methods generally described in Jones, Curr. Opinion Struc. Biol., vol. 7, pp. 377-387, 1997. Such folding can be analyzed based on hydrophobic and/or hydrophilic properties of a target structure.

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One embodiment of the present invention includes a three dimensional computer image of the three dimensional structure of an FCR protein. Suitable structures of which to produce three dimensional computer images are disclosed herein. Preferably, a computer image is created to a structure substantially conforms with the three dimensional coordinates listed in Table 1. A computer image of the present invention can be produced using any suitable software program, including, but not limited to, MOLSCRIPT 2.0 (Avatar Software AB, Heleneborgsgatan 21C, SE-11731 Stockholm, Sweden), the graphical display program 0 (Jones et. al., Acta Crystallography, vol. A47, p. 110, 1991) or the graphical display program GRASP. Suitable computer

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hardware useful for producing an image of the present invention are known to those of skill in the art. Preferred computer hardware includes a Silicon Graphics Workstation.

Another embodiment of the present invention relates to a computer-readable medium encoded with a set of three dimensional coordinates selected from the group of the three dimensional coordinates represented in Table 1, the three dimensional coordinates represented in Table 2, the three dimensional coordinates represented in Table 3, the three dimensional coordinates represented in Table 4, and the three dimensional coordinates represented in Table 5, wherein, using a graphical display software program, the three dimensional coordinates create an electronic file can be visualized on a computer capable of that representing said electronic file as a three dimensional Preferably, the three dimensional structure is of an FcR protein selected from the group of FcyRIIa, FceRI, and FcvRIIIb.

Yet another embodiment of the present invention relates to a computer-readable medium encoded with a set of three dimensional coordinates of a three dimensional structure which substantially conforms to the three dimensional coordinates represented in Table 1, wherein, using a graphical display software program, the set of three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image. Preferably, the three dimensional structure is of an FcR protein selected from the group of FcyRI, FcyRIIa, FcyRIIb, FcyRIIc, FcyRIII, FcgRI and FcqRI.

Another embodiment of the present invention relates to a two dimensional image of an FcR including those illustrated in Fig. 4, Fig. 6, Fig. 7, Fig. 8, Fig. 9, Fig. 10, Fig. 14, Fig. 15 or Fig. 16. Most of these figures

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were drawn with MOLSCRIPT 2.0 (Avatar Software AB, Heleneborgsgatan 21C, SE-11731 Stockholm, Sweden).

One embodiment of the present invention includes an image of FcR protein that is generated when a set of three dimensional coordinates comprising the three dimensional coordinates represented in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of said image and visualizing said electronic file on a computer capable of representing electronic file as a three dimensional image. Suitable graphical software display programs include MOLSCRIPT 2.0, O and GRASP. A suitable computer to visualize such image includes a Silicon Graphics Workstation. structures and models to image are disclosed herein. Preferably, the three dimensional structures and/or models are of an FcR protein selected from the group of FcyRI, FCYRIIa, FCYRIIb, FCYRIIC, FCYRIII, FCERI and FCORI.

present invention also includes three dimensional model of the three dimensional structure of a target structure including FcyRI protein, FcyRIIa, FcyRIIb protein, FcyRIIc protein, FcyRIIIb protein, FceRI protein, and FcaRI protein, such a three dimensional model being produced by the method comprising: (a) providing an amino acid sequences of an FcyRIIa protein and an amino acid sequence of a target FcR structure; (b) identifying structurally conserved regions shared between the FcyRIIa amino acid sequence and the target FcR structure amino acid sequence; (c) determining atomic coordinates for the FcR protein by assigning the structurally conserved regions of the target FcR structure to a three dimensional structure using a three dimensional structure of an FcyRIIa protein based on atomic coordinates that substantially conform to the atomic coordinates represented in Table 1 to derive a model of the three dimensional structure of the target FcR structure amino acid sequence. Preferably, the model

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comprises a computer model. Preferably, the method further comprises the step of electronically simulating the structural assignments to derive a computer model of the three dimensional structure of the target FcR structure amino acid sequence. Preferred amino acid sequences of FcyRI protein, FcyRIIb protein, FcyRIIc protein, FcyRIIIb

protein and FceRI protein are disclosed herein.

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One embodiment of the present invention includes a method for producing crystals of Fc γ RIIa, comprising combining Fc γ RIIa protein with a mother liquor and inducing crystal formation to produce the Fc γ RIIa crystals. Another embodiment of the present invention includes a method for producing crystals of FceRI, comprising combining FceRI protein with a mother liquor and inducing crystal formation to produce the FceRI crystals. Although the production of crystals of Fc γ RIIa and FceRI are specifically described herein, it is to be understood that such processes as are described herein can be adapted by those of skill in the art to produce crystals of other Fc receptors (FcR), particularly Fc γ RI, Fc γ RIIb, Fc γ RIIc, Fc γ RIIIb and Fc α RI, the three dimensional structures of which are also encompassed by the present invention.

Preferably, crystals of FcyRIIa are formed using a solution containing a range of FcyRIIa protein from about 1 mg/ml to about 20 mg/ml, more preferably from about 2 mg/ml to about 15 mg/ml, and even more preferably from about 3 mg/ml to about 6 mg/ml of FcyRIIa protein in a mother liquor, with 3 mg/ml and 6 mg/ml of FcyRIIa protein in a mother liquor being more preferred. Preferably, crystals are formed using droplets containing from about 1 µg to about 30 µg, more preferably from about 5 µg to about 25 µg, and more preferably from about 4.5 µg to about 9 µg of FcyRIIa protein per 3 µl droplet.

A suitable mother liquor of the present invention comprises an acetate salt buffer. A preferred acetate salt

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buffer of the present invention comprises ammonium acetate. The concentration of ammonium acetate in the buffer prior to crystallization can range from about 100 mM to about 500mM ammonium acetate. Preferably, the concentration of ammonium acetate in the buffer ranges from about 150 mM to about 300 mM ammonium acetate. More preferably, the concentration of ammonium acetate in the buffer is 200 $\ensuremath{\mathtt{mM}}$ ammonium acetate. A suitable acetate salt buffer preferably includes a buffer having a pH of from about 5 to about 7, more preferably from about 5.5 to about 6.5, and more preferably a pH of about 5.6. Preferably, the pH of an acetate salt buffer or the present invention is controlled using sodium citrate. A suitable acetate salt buffer contains sodium citrate at a concentration of about 0.01 M sodium citrate, more preferably 0.05 M sodium citrate and more preferably 0.1 M sodium citrate. suitable acetate salt buffer contains any polyethylene glycol (PEG), with PEG 4000 being more preferred. Suitable PEG 4000 concentrations in an acetate salt buffer of the present invention include a concentration of about 20%, preferably about 25%, and more preferably about 30% PEG 4000.

Another suitable mother liquor of the present invention comprises a sulphate buffer. A preferred sulphate buffer of the present invention comprises lithium The concentration of lithium sulfate in the sulfate. buffer prior to crystallization can range from about 100 $\ensuremath{\mathtt{mM}}$ about 2.5 M lithium sulfate. Preferably, concentration of lithium sulfate in the buffer ranges from about 500 mM to about 2 M lithium sulfate. preferably, the concentration of lithium sulfate in the buffer is about 1.5 M lithium sulfate. A suitable sulphate buffer preferably includes a buffer having a pH of from about 5 to about 9, more preferably from about 6 to about 8, and more preferably a pH of about 7.5. Preferably, the

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pH of a sulphate buffer or the present invention is controlled using HEPES. A suitable sulphate buffer contains HEPES at a concentration of about 0.01 M HEPES, more preferably 0.05 M HEPES and more preferably 0.1 M HEPES.

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Supersaturated solutions of FcyRIIa protein can be induced to crystallize by several methods including, but not limited to, vapor diffusion, liquid diffusion, batch crystallization, constant temperature and temperature Preferably, thereof. combination а induction or supersaturated solutions of FcyRIIa protein are induced to crystallize by vapor diffusion (i.e., hanging drop method). In a vapor diffusion method, an FcyRIIa protein is combined with a mother liquor of the present invention that will cause the FcyRIIa protein solution to become supersaturated and form FcyRIIa crystals at a constant temperature. Vapor diffusion is preferably performed under a controlled temperature in the range of from about 15°C to about 30°C, more preferably from about 20°C to about 25°C, and more preferably at a constant temperature of about 22°C.

In a preferred embodiment, the present invention includes a method to produce crystals of FcyRIIa comprising the steps of: (a) preparing an about 3 mg/ml solution of FcyRIIa protein in an acetate salt buffer to form a supersaturated formulation, in which the buffer comprises about 200 mM ammonium acetate, about 100 mM sodium citrate and about 30% PEG 4000 and has a pH of about pH 5.8; (b) dropping about 3 μ l droplets of the supersaturated formulation onto a coverslip and inverting this over a well containing about 1 ml of the acetate salt buffer; and (c) incubating until crystals of FcyRIIa form.

In another preferred embodiment, the present invention includes a method to produce crystals of FcyRIIa comprising the steps of: (a) preparing an about 3 mg/ml solution of FcyRIIa protein in a sulphate buffer to form a

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supersaturated formulation, in which the buffer comprises about 0.15 M HEPES and about 1.5 M lithium sulphate and has a pH of about pH 7.5; (b) dropping about 3 μ l droplets of the supersaturated formulation onto a coverslip and inverting this over a containing about 1 ml of the sulphate buffer; and (c) incubating until crystals of FcyRIIa form.

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As discussed briefly above, another embodiment of the present invention is a method of producing FceRI crystals and the FceRI crystals produced thereby. Preferably, crystals of FceRI are formed using a solution containing a range of FceRI protein from about 1 mg/ml to about 20 mg/ml, more preferably from about 2 mg/ml to about 15 mg/ml, and even more preferably from about 3 mg/ml to about 6 mg/ml of FceRI protein in a mother liquor, with 3 mg/ml and 6 mg/ml of FceRI protein in a mother liquor being more preferred. Preferably, crystals are formed using droplets containing from about 1 µg to about 30 µg, more preferably from about 5 µg to about 25 µg, and more preferably from about 4.5 µg to about 9 µg of FceRI protein per 3 µl droplet.

A suitable mother liquor of the present invention comprises an acetate salt buffer. A preferred acetate salt buffer of the present invention comprises calcium acetate. The concentration of calcium acetate in the buffer prior to crystallization can range from about 100 mM to about 500 mM $\,$ calcium acetate. Preferably, the concentration of calcium acetate in the buffer ranges from about 150 mM to about 300 $\,$ mM calcium acetate. More preferably, the concentration of calcium acetate in the buffer is 200 mM calcium acetate. A suitable acetate salt buffer preferably includes a buffer having a pH of from about 5.5 to about 7.5, more preferably from about 6.0 to about 7.0, and more preferably a pH of about 6.5. Preferably, the pH of an acetate salt buffer or the present invention controlled is using sodium cacodylate. A suitable acetate salt buffer contains sodium

cacodylate at a concentration of about 0.01 M sodium

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cacodylate, more preferably 0.05 M sodium cacodylate and more preferably 0.1 M sodium cacodylate. A suitable acetate salt buffer contains any polyethylene glycol (PEG), with PEG 8000 being more preferred. Suitable PEG 8000 concentrations in an acetate salt buffer of the present invention include a concentration of about 10% w/v, preferably about 15%, and more preferably about 20% w/v PEG

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10 Another suitable mother liquor of the present invention comprises a buffer which includes cacodylate together with 2-propanol and polyethylene A preferred sodium cacodylate buffer of the glycol. present invention comprises a concentration of sodium cacodylate in the buffer prior to crystallization of about 15 0.01 M sodium cacodylate, more preferably 0.05 M sodium cacodylate and more preferably 0.1 M sodium cacodylate. A suitable sodium cacodylate buffer preferably includes a buffer having a pH of from about 5 to about 7, more preferably from about 5.5 to about 6.5, and more preferably 20 a pH of from about 5.5 to about 6.0. A suitable sodium cacodylate buffer contains 2-propanol at a concentration of about 5% v/v, more preferably 7% v/v and more preferably 10% v/v. A suitable sodium cacodylate buffer contains any polyethylene glycol (PEG), with PEG 4000 being more 25 preferred. Suitable PEG 4000 concentrations in an acetate buffer of the present invention include concentration of about 10% w/v, preferably about 15%, and more preferably about 20% w/v PEG 4000.

Another suitable mother liquor of the present invention comprises a sodium citrate buffer which includes tri sodium citrate dihydrate together with sodium cacodylate and 2-propanol. A preferred sodium citrate buffer of the present invention comprises a concentration of tri sodium citrate dihydrate in the buffer prior to

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crystallization of about 0.05 M tri sodium dihydrate, more preferably 0.1 M tri sodium citrate dihydrate and more preferably 0.2 M tri sodium citrate dihydrate. A suitable sodium citrate buffer preferably includes a buffer having a pH of from about 5.5 to about 7, more preferably from about 6.0 to about 7.0, and more preferably a pH of about 6.5. A preferred sodium citrate buffer of the present invention comprises a concentration of sodium cacodylate in the buffer prior to crystallization of about 0.01 M sodium cacodylate, more preferably 0.05 M sodium cacodylate and more preferably 0.1 M sodium cacodylate. A suitable sodium citrate buffer contains 2propanol at a concentration of about 15% v/v, more preferably 20% v/v and more preferably 30% v/v.

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Supersaturated solutions of FceRI protein can be induced to crystallize by several methods including, but not limited to, vapor diffusion, liquid diffusion, batch crystallization, constant temperature and temperature induction or a combination thereof. Preferably, supersaturated solutions of FceRI protein are induced to crystallize by vapor diffusion (i.e., hanging drop method). In a vapor diffusion method, an FceRI protein is combined with a mother liquor of the present invention that will cause the FceRI protein solution to become supersaturated and form FceRI crystals at a constant temperature. diffusion is preferably performed under a controlled temperature in the range of from about 15°C to about 30°C, more preferably from about 20°C to about 25°C, and more preferably at a constant temperature of about 22°C.

In a preferred embodiment, the present invention includes a method to produce crystals of FceRI comprising the steps of: (a) preparing an about 3 mg/ml solution of FceRI protein in an acetate salt buffer to form a supersaturated formulation, in which the buffer comprises about 200 mM calcium acetate, about 100 mM sodium

cacodylate and about 18% w/v PEG 8000 and has a pH of about pH 6.5; (b) dropping about 3 μ l droplets of the supersaturated formulation onto a coverslip and inverting this over a well containing about 1 ml of the acetate salt buffer; and (c) incubating until crystals of FceRI form.

In another preferred embodiment, the present invention includes a method to produce crystals of FceRI comprising the steps of: (a) preparing an about 3 mg/ml solution of FceRI protein in a sodium cacodylate buffer to form a supersaturated formulation, in which the buffer comprises about 100 mM sodium cacodylate, about 10% v/v 2-propanol and about 20% w/v PEG 4000 and has a pH of about pH 5.5-6.0; (b) dropping about 3 μ l droplets of the supersaturated formulation onto a coverslip and inverting this over a containing about 1 ml of the sulphate buffer; and (c) incubating until crystals of FceRI form.

In another preferred embodiment, the present invention includes a method to produce crystals of FceRI comprising the steps of: (a) preparing an about 3 mg/ml solution of FceRI protein in a sodium citrate buffer to form a supersaturated formulation, in which the buffer comprises about 200 mM tri sodium citrate dihydrate, about 100 mM sodium cacodylate and about 30% v/v 2-propanol and has a pH of about pH 6.5; (b) dropping about 3 μ l droplets of the supersaturated formulation onto a coverslip and inverting this over a containing about 1 ml of the sulphate buffer; and (c) incubating until crystals of FceRI form.

Any isolated FcR protein can be used with the present method. An isolated FcR protein can be isolated from its natural milieu or produced using recombinant DNA technology (e.g., polymerase chain reaction (PCR) amplification, cloning) or chemical synthesis. To produce recombinant FcR protein, a nucleic acid molecule encoding FcR protein can be inserted into any vector capable of delivering the nucleic acid molecule into a host cell. Suitable and

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preferred nucleic acid molecules to include in recombinant vectors of the present invention are as disclosed herein. A preferred nucleic acid molecule of the present invention encodes a human FcR protein, and more preferably, a human FcyRIIa protein, a human FceRI protein, or a human FcyRIIIb protein. A nucleic acid molecule of the present invention can encode any portion of an FcR protein, preferably a full-length FcR protein, and more preferably a soluble form of FcR protein (i.e., a form of FcR protein capable of being secreted by a cell that produces such protein). more preferred nucleic acid molecule to include in a recombinant vector, and particularly in a recombinant molecule, includes a nucleic acid molecule encoding a protein having the amino acid sequence represented by SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, or SEQ ID NO:13. A preferred nucleic acid molecule to include in a recombinant molecule includes sFcyRIIa and sFceRI, the production of which are described in the Examples section.

A recombinant vector of the present invention can be either RNA or DNA, either prokaryotic or eukaryotic, and typically is a virus or a plasmid. Preferably, a nucleic acid molecule encoding an FcR protein is inserted into a vector comprising an expression vector to recombinant molecule. As used herein, an expression vector is a DNA or RNA vector that is capable of transforming a host cell and of affecting expression of a specified nucleic acid molecule. Expression vectors of the present invention include any vectors that function (i.e., direct gene expression) in recombinant cells of the present invention, including in bacterial, fungal, endoparasite, insect, other animal, and plant cells. Preferred expression vectors of the present invention direct expression in insect cells. A more preferred expression

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vector of the present invention comprises pVL1392 baculovirus shuttle plasmid. A preferred recombinant molecule of the present invention comprises pVL-sFcyRIIa(a), pVL-sFcyRIIa(b), and pVL-sFceRI.

An expression vector of the present invention can be into any suitable host cell to form a transformed recombinant cell. A suitable host cell includes any cell capable of expressing a nucleic acid molecule inserted into a prokaryotic For example, the expression vector. expression vector can be transformed into a bacterial host A preferred host cell of the present invention includes a cell capable of expressing a baculovirus, in particular an insect cell, with Spodoptera frugiperda or A preferred Trichoplusia ni cells being preferred. recombinant cell of the present invention includes S. $frugiperda: pVL-sFc\gamma RIIa(a) / pVL-sFc\gamma RIIa(b)$ cells and S.frugiperda:pVL-sFccRI the production of which is described herein.

One method to isolate FcR protein useful for producing FcR crystals includes recovery of recombinant proteins from cell cultures of recombinant cells expressing such FcR In one embodiment, an isolated recombinant FcR protein. protein of the present invention is produced by culturing a cell capable of expressing the protein under conditions effective to produce the protein, and recovering the protein. A preferred cell to culture is a recombinant cell Effective culture conditions of the present invention. but are not limited to, effective media, include, bioreactor, temperature, pH and oxygen conditions and culture medium that permit protein production. Such culturing conditions are within the expertise of one of ordinary skill in the art. Examples of suitable conditions are included in the Examples section.

Preferably, a recombinant cell of the present invention expresses a secreted form of FcR protein. FcR

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proteins of the present invention can be purified using a variety of standard protein purification techniques, such as, but not limited to, affinity chromatography, ion exchange chromatography, filtration, electrophoresis, hydrophobic interaction chromatography, gel filtration chromatography, phase reverse chromatography, chromatofocusing differential and solubilization. Preferably, an FcR protein is purified in such a manner that the protein is purified sufficiently for formation of crystals useful for obtaining information related to the three dimensional structure of an FcR protein. Preferably, a composition of FcR protein is about 70%, more preferably 75%, more preferably 80%, more preferably 85% and more preferably 90% pure.

In one embodiment, a recombinant FcR protein is purified from a cell culture supernatant harvested between about 20 hours and about 60 hours post-infection, preferably between about 30 hours and about 50 hours post-infection, and more preferably about 40 post-infection. Preferably, an FcyRIIa protein is purified from a supernatant by a method comprising the steps: (a) supernatant from s . applying frugiperda:pVL-sFcyRIIa(a)/pVL-sFcyRIIa(b) cells to an ion exchange column; (b) collecting unbound protein from the ion exchange column and applying the unbound protein to an immuno-affinity chromatography column; (c) eluting proteins bound to the immuno-affinity chromatography column and applying the eluted proteins to a gel filtration column; and (d) collecting filtered proteins from the filtration column to obtain the FcyRIIa protein. Preferably, an FceRI protein is purified from a supernatant by a method comprising the steps: (a) applying supernatant from S. frugiperda:pVL-sFccRI cells to an ion exchange (b) collecting unbound protein from the ion column: exchange column and applying the unbound protein to an

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immuno-affinity chromatography column; (c) eluting proteins bound to the immuno-affinity chromatography column and applying the eluted proteins to a gel filtration column; and (d) collecting filtered proteins from the gel filtration column to obtain the FceRI protein.

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In view of the high degree of amino acid sequence homology between human $Fc\gamma R$ proteins and other members of the $Fc\gamma R$ family of proteins, the methods of purification of the present invention are applicable for each member of the FcyR family. In addition, one of skill in the art will recognize that the purification methods of the present invention are generally useful for purifying any FcR protein, such as the FceRI protein, except using IgE rather than IgG for the step of immuno-affinity chromatography purification, and such as the Fc α RI protein, except using IgA rather than IgG for the purification step. Isolated protein of the members of the Fc γ R family of proteins, Fc ε R protein and $Fc\alpha R$ protein may be obtained through recombinant DNA technology or may be purified from natural sources, including but not limited to, monocytes, macrophages, neutrophils, eosinophils, platelets and B lymphocytes (i.e., B cells). Descriptions of recombinant production of isolated FcyRIIa and FceRI proteins are described in the Examples section.

Another embodiment of the present invention includes a composition comprising FcR protein in a crystalline form (i.e., FcR crystals). As used herein, the terms "crystalline FcR" and "FcR crystal" both refer to crystallized FcR protein and are intended to be used interchangeably. Preferably, a crystalline FcR is produced using the crystal formation method described herein, in particular according to the method disclosed in Example 6 or Example 9. A FcR crystal of the present invention can comprise any crystal structure and preferably precipitates as an orthorhombic crystal. A suitable crystalline FcR of

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the present invention includes a monomer or a multimer of FcR protein. A preferred crystalline FcR comprises one FcR protein in an asymmetric unit. A more preferred crystalline FcR comprises a dimer of FcR proteins.

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A particular embodiment of the present invention includes a composition comprising FcyRIIa protein in a crystalline form (i.e., FcyRIIa crystals). As used herein, the terms "crystalline FcYRIIa" and "FcYRIIa crystal" both refer to crystallized FcYRIIa protein and are intended to be used interchangeably. Preferably, a crystal FcyRIIa is produced using the crystal formation method described herein, in particular according to the method disclosed in Example 6. A FcyRIIa crystal of the present invention can comprise any crystal structure and preferably precipitates as an orthorhombic crystal. Preferably, a composition of the present invention includes $Fc\gamma RIIa$ protein molecules arranged in a crystalline manner in a space group $P2_12_12_1$, so as to form a unit cell of dimensions a = 78.80 Å, b = 100.55 Å, c = 27.85 Å. A preferred crystal of the present invention provides X-ray diffraction data for determination of atomic coordinates of the $Fc\gamma RIIa$ protein to a resolution of about 3.0 Å, preferably about 2.4 Å, and more preferably at about 1.8 Å.

A suitable crystalline FcYRIIa of the present invention includes a monomer or a multimer of FcYRIIa protein. A preferred crystalline FcYRIIa comprises one FcYRIIa proteins in an asymmetric unit. A more preferred crystalline FcYRIIa comprises a dimer of FcYRIIa proteins.

Another particular embodiment of the present invention includes a composition comprising FceRI protein in a crystalline form (i.e., FceRI crystals). As used herein, the terms "crystalline FceRI" and "FceRI crystal" both refer to crystallized FceRI protein and are intended to be used interchangeably. Preferably, a crystal FceRI is produced using the crystal formation method described

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herein, in particular according to the method disclosed in Example 9. A FceRI crystal of the present invention can comprise any crystal structure and preferably precipitates as an orthorhombic crystal. A suitable crystalline FceRI of the present invention includes a monomer or a multimer of FceRI protein. A preferred crystalline FceRI comprises one FceRI protein in an asymmetric unit. A more preferred crystalline FceRI comprises a dimer of FceRI proteins.

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According to the present invention, crystalline FcR can be used to determine the ability of a chemical compound of the present invention to bind to FcyRIIa protein a manner predicted by a structure based drug design method of the present invention. Preferably, an FcyRIIa crystal is soaked in a solution containing a chemical compound of the present invention. Binding of the chemical compound to the crystal is then determined by methods standard in the art.

One embodiment of the present invention is a therapeutic composition. A therapeutic composition of the present invention comprises one or more therapeutic compounds. Preferred therapeutic compounds of the present invention include inhibitory compounds and stimulatory compounds.

invention One embodiment of the present capable of reducing therapeutic composition that is therapeutic Suitable damage. IgG-mediated tissue compositions are capable of reducing IgG-mediated tissue damage resulting from IgG-mediated hypersensitivity or other biological mechanisms involved in IgG-mediated recruitment of inflammatory cells that involves FcYR protein. For example, a therapeutic composition of the present invention can: (1) inhibit (i.e., prevent, block) binding of FcyR protein on a cell having an FcyR protein (e.g., B cells, macrophage, neutrophil, eosinophil or platelet cells) to an IgG immune complex by interfering with the IgG binding site of an FcyR protein; (2) binding

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to the Fc portion of IgG to inhibit complement fixation by an IgG immune complex by interfering with the complement binding site of an IgG molecule; (3) inhibit precipitation of IgG or IgG immune complexes (i.e., prevent Fc:Fc interactions between two IqG); (4)inhibit immunoglobulin-mediated cellular signal transduction by interfering with the binding of an IgG to a cell surface receptor; (5) inhibit FcYR-mediated cellular signal transduction by interfering with the binding of a cell signal inducing molecule (i.e., a molecule that induces cellular signal transduction through an FcyR protein) to an FcyR protein; (6) inhibit opsinization of pathogens by inhibiting binding of IgG bound to a pathogen to FcYR protein on a phagocytic cell (e.g., to prevent antibody dependent enhancement (ADE) of viral infection, such as with flaviviruses and dengue virus); and (7) inhibit the binding of viral molecules to FcyR protein (e.g., measles virus nucleocapsid protein). As used herein, the term "immune complex" refers to a complex that is formed when an antibody binds to a soluble antigen. As used herein, the term "complement fixation" refers to complement activation by an antigen: antibody complex that results in recruitment of inflammatory cells, typically by assembly of a complex comprising C3a and C5a, or generation of cleaved C4. used herein, the term "binding site" refers to the region of a molecule (e.g., a protein) to which another molecule specifically binds. Such therapeutic compositions include one or more inhibitory compounds that inhibit binding of IgG to FcyR protein, IgG to complement, IgG to IgG, IgG to a cell surface receptor, a cell signal inducing molecule to protein, FcyR protein to virus opsinization. Also included in the present invention are methods to reduce IgG-mediated tissue damage. The method includes the step of administering to an animal a therapeutic composition of the present invention.

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Another embodiment of the present invention is a therapeutic composition that is capable of stimulating an IgG humoral immune response in an animal. Yet another embodiment of the present invention is a therapeutic composition that improves the therapeutic affects of an antibody that is administered to an animal to treat, by opsinization or FcyR-dependent effector functions (e.g. antibody-dependent FcyR-medicated cytotoxicity, phagocytosis or release of cellular mediators), particular disease, including, but not limited to, cancer or infectious disease (e.g. oral infections such as HIV, herpes, bacterial infections, yeast infections or parasite infections). Such a therapeutic composition includes one or more stimulatory compounds that have increased binding to IgG, enhance binding of IgG to Fc γR , enhance dimer formation of an $Fc\gamma R$ and/or enhance signal transduction through the FcYR. Also included in the present invention is a method to stimulate a humoral immune response. The method includes the step of administering to an animal a therapeutic composition of the present invention.

Suitable inhibitory compounds of the present invention are compounds that interact directly with an FcyR protein, preferably an FcyRIIa protein or an FcyRIIIb protein, thereby inhibiting the binding of IgG to an FcyR protein, by either blocking the IgG binding site of an FcyR (referred to herein as substrate analogs) or by modifying other regions of the FcyR protein (such as in the upper groove of the IgG binding cleft between the monomers of an FcyR dimer, at the dimer interface, in the cleft or hinge region between D1 and D2 on each monomer, and/or underneath the IgG binding cleft in the lower groove formed by the monomers of an FcyR dimer) such that IgG cannot bind to the FcyR (e.g., by allosteric interaction). A FcyR substrate analog refers to a compound that interacts with (e.g., binds to, associates with, modifies) the IgG binding site

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of an FcyR protein. A FcyR substrate analog can, for example, comprise a chemical compound that mimics the Fc portion of an IgG, or that binds specifically to the IgG binding site of an FcyR but does not mimic the Fc portion of an IgG. An inhibitory compound of the present invention can also include a compound that essentially mimics at least a portion of an FcyRIIa protein that binds to IgG (referred to herein as a peptidomimetic compound). suitable inhibitory compounds of the present Other invention include compounds that inhibit the binding of an FcyR protein to a cell signal inducing molecule other than Examples of such cell signal inducing molecules include another FcyR (i.e., to form a dimer of FcyR proteins), or a cell surface accessory molecule, an intracellular accessory molecule or virus (e.g., measles virus nucleocapsid protein).

One embodiment of the present invention therapeutic composition that is capable of reducing IgE-mediated responses. Suitable therapeutic compositions are capable of reducing IgE-mediated responses resulting from IgE-mediated hypersensitivity, IgE-mediated release of inflammatory modulators or other biological mechanisms involved in IgE-mediated recruitment of inflammatory cells that involves FceR protein. For example, a therapeutic composition of the present invention can: (1) inhibit (i.e., prevent, block) binding of FceR protein on a cell having an FceR protein (e.g., mast cells) to an IgE immune complex by interfering with the IgE binding site of an FceR protein; (2) inhibit precipitation of IgE or IgE immune complexes (i.e., prevent Fc:Fc interactions between two IqE); (3) inhibit immunoqlobulin-mediated cellular signal transduction by interfering with the binding of an IgE to a cell surface receptor; and (4) inhibit FceR-mediated cellular signal transduction by interfering with the binding of a cell signal inducing molecule (i.e., a

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molecule that induces cellular signal transduction through an FceR protein) to an FceR protein. Such therapeutic compositions include one or more inhibitory compounds that inhibit binding of IgE to FceR protein, IgE to IgE, IgE to a cell surface receptor, or a cell signal inducing molecule to FceR protein. Also included in the present invention are methods to reduce IgE-mediated responses, such as IgE-mediated inflammation. The method includes the step of administering to an animal a therapeutic composition of the present invention.

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Another embodiment of the present invention is a therapeutic composition that is capable of stimulating a IgE humoral immune response in an animal. Yet another embodiment of the present invention is a therapeutic composition that improves the therapeutic affects of an antibody that is administered to an animal to treat, by opsinization or FceR-dependent effector functions (e.g. phagocytosis or release of cellular mediators), particular disease. Such a therapeutic composition includes one or more stimulatory compounds that have increased binding to IgE, enhance binding of IgE to FceRI, enhance dimer formation of FccRI and/or otherwise enhance signal transduction through the FceRI. Also included in the present invention is a method to stimulate a humoral immune response. The method includes the administering to an animal a therapeutic composition of the present invention.

Suitable inhibitory compounds of the present invention are compounds that interact directly with an FceR protein, thereby inhibiting the binding of IgE to an FceR protein, by either blocking the IgE binding site of an FceR (referred to herein as substrate analogs) or by modifying other regions of the FceR protein (such as in the upper groove of the IgE binding cleft between the monomers of an FceRI dimer, at the dimer interface, in the cleft or hinge

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region between D1 and D2 on each monomer, and/or underneath the IgE binding cleft in the lower groove formed by the monomers of an FceRI dimer) such that IgE cannot bind to the FceR (e.g., by allosteric interaction). A FCER substrate analog refers to a compound that interacts with (e.g., binds to, associates with, modifies) the IgE binding site of an FceR protein. A FceR substrate analog can, for example, comprise a chemical compound that mimics the Fc portion of an IgE, or that binds specifically to the IgE binding site of an FceR but does not mimic the Fc portion of an IgE. An inhibitory compound of the present invention can also include a compound that essentially mimics at least a portion of an FceR protein that binds to IgE (referred to herein as a peptidomimetic compound). Other suitable inhibitory compounds of the present invention include compounds that inhibit the binding of an FceR protein to a cell signal inducing molecule other than Examples of such cell signal inducing molecules include another FceR (i.e., to form a dimer of FceR proteins), or a cell surface accessory molecule, intracellular accessory molecule or virus (e.g., measles virus nucleocapsid protein).

Inhibitory compounds of the present invention can be identified by various means known to those of skill in the For example, binding of an inhibitory compound to, or otherwise interaction with, an FcR protein, determined with FcR protein in solution or on cells using, for example, immunoassays such as enzyme linked immunoabsorbent assays (ELISA) and radioimmunoassays (RIA) or binding assays such as Biacore assays. assays can include, for example, cytokine (e.g., IL-4, IL-6 IL-12) secretion assays, or intracellular signal transduction assays that determine, for example, protein or lipid phosphorylation, mediator release or intracellular

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 $\text{Ca}^{\text{++}}$ mobilization upon FcR binding to a cell signal inducing molecule.

Suitable stimulatory therapeutic compounds of the present invention are compounds that exhibit improved binding to Ig when compared with the ability of a natural FcR protein (e.g., an FcR protein isolated from its natural milieu) to bind to Ig, and also include compounds that enhance the binding of Ig to its FcR or enhance signal transduction through the FcR. Stimulatory compounds of the present invention are identified by their ability to: (1) bind to, or otherwise interact with, Ig at a higher level than, for example, natural FcR protein; (2) enhance binding of Ig to its FcR; (3) enhance dimer formation of an FcR by binding either to the FcR, to an Ig that binds to the FcR or to the combination of Ig bound to the FcR; and/or (4) enhance signal transduction through the FcR. determine improved binding of Ig to a stimulatory compound of the present invention compared with, for example, natural FcR protein, include binding assays that determine the stability of binding, affinity or kinetics at which an Ig binds to a stimulatory compound and a natural FcR protein. Such methods are well known to those of skill in the art and are disclosed herein in the Examples section. A stimulatory compound of the present invention can also include a compound that binds to an Ig or an FcR protein, thereby enhancing the binding of Ig to FcR protein or improving cellular signal transduction during or after the binding of Ig to FcR protein, by, for example, modifying other regions of the FcR or Ig by an allosteric interaction that modifies the Ig-binding site of FcR or the Fc portion of Ig that binds to an FcR protein. Another stimulatory compound of the present invention can include a compound that binds to FcR protein in the absence of Ig, in such a manner that FcR-mediated cellular signal transduction is stimulated.

One of skill in the art will understand that inhibitory or stimulatory compounds can also be developed based on the structure of any FcR and its Ig ligand, as described above for FcyR protein and IgG and FceRI and IgE.

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According to the present invention, suitable therapeutic compounds of the present invention include peptides or other organic molecules, and inorganic Suitable organic molecules include molecules. organic molecules. Preferably, a therapeutic compound of the present invention is not harmful (e.g., toxic) to an animal when such compound is administered to an animal. Peptides refer to a class of compounds that is small in molecular weight and yields two or more amino acids upon hydrolysis. A polypeptide is comprised of two or more peptides. As used herein, a protein is comprised of one or more polypeptides. Preferred therapeutic compounds to design include peptides composed of "L" and/or "D" amino acids that are configured as normal or retroinverso peptides, peptidomimetic compounds, small molecules, or homo- or hetero-polymers thereof, in linear or branched configurations.

Therapeutic compounds of the present invention can be designed using structure based drug design. Until the discovery of the three dimensional structure of the present invention, no information was available for structure based development of therapeutic compounds based on the structure of FcR protein. Such rational development heretofore could not be executed de novo from available linear amino acid sequence information. Structure based drug design refers to the use of computer simulation to predict a conformation of a peptide, polypeptide, protein, or conformational interaction between a peptide or polypeptide, therapeutic compound. For example, generally, for a protein to effectively interact with a therapeutic compound, it is necessary that the three dimensional

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structure of the therapeutic compound assume a compatible conformation that allows the compound to bind to the protein in such a manner that a desired result is obtained

upon binding. Knowledge of the three dimensional structure of the protein enables a skilled artisan to

design a therapeutic compound having such compatible

conformation. For example, knowledge of the three

dimensional structure of the IgG binding site of $Fc\gamma RIIa$ protein enables one of skill in the art to design a

therapeutic compound that binds to FcyRIIa, is stable and

results in inhibition of a biological response such as IgG

binding to cells having $Fc\gamma R$, or cellular signal

transduction, upon such binding. In addition, for example,

knowledge of the three dimensional structure of the IgG binding site of Fc γ RIIa protein enables a skilled artisan

to design a substrate analog of FcyRIIa protein.

Suitable structures and models useful for structure based drug design are disclosed herein. Preferred structures to use in a method of structure based drug design include a structure of FcyRIIa protein, a structure of FceRI protein, a structure of an FcyRIIIb protein, and a model of a target FcR structure. Preferred models of target structures to use in a method of structure based drug design include models produced by any modeling method disclosed herein, including molecular replacement and fold recognition related methods.

One embodiment of the present invention is a computer-assisted method of structure based drug design of bioactive compounds, comprising: (a) providing a structure of a protein including a three dimensional structure of an FCR protein or a model of the present invention; (b) designing a chemical compound using the three dimensional structure or model; and (c) chemically synthesizing the chemical compound. Such a method can additionally include the step of (d) evaluating the bioactivity of the

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synthesized chemical compound. Suitable three dimensional structures an FcR protein and models to use with the present method are disclosed herein. According to the present invention, the step of designing can include creating a new chemical compound or searching databases of libraries of known compounds (e.g., a compound listed in a screening database containing computational dimensional structures of known compounds). Designing can also be performed by simulating chemical compounds having substitute moieties at certain structural features. step of designing can include selecting a chemical compound based on a known function of the compound. step of designing comprises computational screening of one more databases of compounds in which the three dimensional structure of the compound is known and is interacted (e.g., docked, aligned, matched, interfaced) with the three dimensional structure of an FcR protein by computer (e.g. as described by Humblet and Dunbar, Animal Reports in Medicinal Chemistry, vol. 28, pp. 275-283, 1993, M Venuti, ed., Academic Press). Methods to synthesize suitable chemical compounds are known to those of skill in the art and depend upon the structure of the chemical being Methods to evaluate the bioactivity of the synthesized. synthesized compound depend upon the bioactivity of the inhibitory or stimulatory) compound (e.q., disclosed herein.

Various other methods of structure-based drug design are disclosed in Maulik et al., 1997, Molecular Biotechnology: Therapeutic Applications and Strategies, Wiley-Liss, Inc., which is incorporated herein by reference in its entirety. Maulik et al. disclose, for example, methods of directed design, in which the user directs the process of creating novel molecules from a fragment library of appropriately selected fragments; random design, in which the user uses a genetic or other algorithm to

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randomly mutate fragments and their combinations while simultaneously applying a selection criterion to evaluate the fitness of candidate ligands; and a grid-based approach in which the user calculates the interaction energy between three dimensional receptor structures and small fragment probes, followed by linking together of favorable probe sites.

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Preferably, a chemical compound of the present invention that binds to the Ig binding site of an FcR protein is known to originate from a chemical compound having chemical and/or stereochemical complementarity with protein and/or Iq. Such complementarity characteristic of a chemical compound that matches the surface of the receptor either in shape or in distribution of chemical groups and binds to FcR protein to promote or inhibit Ig binding to the FcR protein, or to induce cellular signal transduction upon binding to FcR protein. More preferably, a chemical compound that binds to the Ig binding site of an FcR protein associates with an affinity of at least about $10^{-6}\ \mathrm{M},$ and more preferably with an affinity of at least about $10^{-8}\ \mathrm{M}.$

Preferably, five sites of FcR protein are targets for structure based drug design. These sites include the Ig-binding site of FcR protein, the upper groove between two FcR monomers, the dimerization interface between two FcR protein monomers, the lower groove between two FcR monomers, the interface, cleft or hinge region between Domains 1 and 2 of FcR protein, and combinations of any of these sites (e.g., interacting with the Ig-binding site and the upper groove between monomers simultaneously). A schematic representation of these sites is shown in Fig. 17, with "a" representing the Ig-binding site of FcR protein, "b" representing the upper groove between two FcR monomers, "c" representing the dimerization interface between two FcR protein monomers, "d" representing the

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interface, cleft or hinge region between Domains 1 and 2 of FcR protein, and "e" representing the lower groove between The following discussion provides two FcR monomers. specific detail on drug-design using target sites of the FcR and as an example, references preferred target sites on It is to be understood, however, the FcyRIIa structure. that one of skill in the art, using the description of the FceRI structure and the FcyRIIIb structure provided herein, will be able to effectively select similar target sites on the FceRI protein monomer and dimer for structure based drug design. Additionally, one of skill in the art, now being able to model the other FcR proteins based on the information provided herein, will also be effectively select similar target sites on the other FcR proteins for structure based drug design.

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The Ig-binding site (Fig. 17; "a") is targeted to directly affect the binding of FcR to Ig (i.e., inhibition The IgG binding site of FcyRIIa protein, or enhancement). for example, includes, but is not limited to, residues 155, 156, 158-160, 113-116 , 129, 131, 133 and 134 of SEQ ID NO:3, and can also include at least a portion of the second site described above (Fig. 17; "b"), the groove between the two IgG binding sites that form upon dimerization of FcyRIIa protein. Residues from site "b" that are included in IgG binding include, but are not limited to, residues 117-121, 125-129, 150-154 and 157-161 of SEQ ID NO:3. suitable target site for structure based drug design comprising the IgG binding site of FcyRIIa protein is illustrated in Fig. 7. More specifically, mutagenesis studies have identified several residues which have an effect on the binding of IgG, and the three dimensional structure disclosed herein clearly identifies which surface exposed (i.e., are likely to residues are participate in binding of IgG and are not just having an allosteric effect). These residues can be classified in

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three spatial groups: (1) Phe129, His131, Lys113, Pro114, Leu115, Vall16; (2) Pro134 and Asp133; and (3) Leu159 and Ser161. Group (1) forms a continuous surface leading from the lip of the groove "b" (Fig. 17) across the binding surface "a" (Fig. 17), and represents the most preferred target of design work at the site of IgG binding. Group (2) is separated from Group (1) by Leu132, which is currently of unknown importance in the binding of IgG, and may well be part of the surface exposed residues. Group (3) contains residues which are remote from the other two groups and do not appear to be available to participate in binding of the IgG by the dimer structure.

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The upper groove between the two monomers of the FcR (Fig. 17; "b") is also targeted to directly affect the binding of FcR to Ig (i.e., inhibition or enhancement). The upper groove provides an attractive site to build into in contrast to targeting a flat protein surface. The dimer structure of the FcyRIIa protein suggests targeting C2 or pseudo C2 symmetric inhibitors. Preferred residues to target in the FcyRIIa protein include Lys117, His131, Phe129, Asn154, Ser161, Leu159, Thr152 and Phe121, with Phe129, Lys117 and His131 being most preferred. embodiment, compounds can be designed which interact with both the upper groove "b" and the IgG binding surface "a" simultaneously. For example, improved Ig regulatory compounds may be obtained by designing regulatory compounds which flow out of the groove and bind to the binding surface of "a" as described above. Alternatively, regulatory compound which binds to "b" may sterically hinder binding of IgG to "a" without actually interacting with the "a" binding surface.

The receptor dimer interface (Fig. 17; "c") is targeted to directly affect the ability of two FcR proteins to form a dimer, thereby affecting cellular signal transduction through one or both of the FcR proteins.

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Without being bound by theory, the present inventors believe that dimer formation can affect cellular signal transduction or affect the conformation of the Ig binding of one or both of the FcR proteins involved in the dimer, thereby affecting cellular signal transduction. addition, the dimer interface represents an excellent target site because one monomer provides ligand information for the other monomer and vice versa. A suitable target site for structure based drug design comprising the dimerization interface between two FcyRIIa proteins is illustrated in Fig. 10. More specifically, residues 117-131 and residues 150-164 make up the interfacial area of the FcyRIIa dimer, and peptides from these sequences or their mimics may be binding inhibitors. An examination of hydrogen bonding interactions from the crystal structure of $Fc\gamma RIIa$ indicates relatively few interactions between the monomers in the interfacial area, but a notable cluster is spanned by the hexapeptide Phel21-Gln122-Asn123-Gly124-Lys125-Ser126. Additionally, there is a hydrogen bond between the monomers involving Gly124-Ser561 and Ser126-Leu559. There are also some hydrophobic contacts made by the Lys125 sidechain and by the Phel21 phenyl ring.

The interface between Domains 1 and 2 (Fig. 17; "d") is targeted to affect IgG binding to an FcyRIIa protein. The present inventors have discovered that in the three dimensional structure of FcyRIIa protein, Domain 1 makes close contact with Domain 2. In particular, a loop comprising residues 17-20 of SEQ ID NO:3 in Domain 1 lie close to the loops of Domain 2 to form at least a portion of the IgG-binding site. Interactions with IgG are believed to occur close to the D1D2 interface and so alterations at this site mav effect Iq Additionally, a cleft is defined by residues 12-14 (base), 6-10 and 77-80 (D1 face) and 93-96 and 101 (D2 face), and as such represents a potential site for inhibitor design.

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A suitable target site for structure based drug design comprising the interface between Domain 1 and Domain 2 of an FcyRIIa protein is illustrated in Fig. 5.

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The lower groove between the two monomers of the FcR (Fig. 17; "e") is also targeted to directly affect the binding of FcR to Ig (i.e., inhibition or enhancement). A similar design strategy can be used for this site as described above for the upper groove "b", although it is less clear whether compounds binding to this site would be inhibitory, or more probably enhance IgG binding to the FcyR.

Drug design strategies as specifically described above with regard to residues and regions of the FcyRIIa monomer and dimer can be similarly applied to the other FcR structures, including the FcYRIIIb and FceRI structures disclosed herein. One of ordinary skill in the art, using the art recognized modeling programs and drug design methods, many of which are described herein, will be able modify the FcyRIIa design strategy according to differences in amino acid sequence and more favored structures, for example, in the other FcR, to similarly design compounds which regulate other FcR action. addition, one of skill in the art could use lead compound structures derived from one FcR, such as the FcyRIIa protein, and taking into account differences in amino acid residues in another FcR protein, such as FceRI, modify the FcyRIIa lead compound to design lead compound structures for regulation of the FceRI protein. For example, His131>Tyr131 in the upper groove pharmacophore could be accommodated by changing an acidic moiety in an Fc γ RIIa lead compound structure to an electron deficient ketone moiety.

In the present method of structure based drug design, it is not necessary to align a candidate chemical compound (i.e., a chemical compound being analyzed in, for example,

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a computational screening method of the present invention) to each residue in a target site. Suitable candidate chemical compounds can align to a subset of residues described for a target site. Preferably, a candidate chemical compound comprises a conformation that promotes the formation of covalent or noncovalent crosslinking between the target site and the candidate chemical compound. Preferably, a candidate chemical compound binds to a surface adjacent to a target site to provide an additional site of interaction in a complex. designing an antagonist (i.e., a chemical compound that inhibits the binding of a ligand to FcR protein by blocking a binding site or interface), the antagonist should bind with sufficient affinity to the binding site or to substantially prohibit a ligand (i.e., a molecule that specifically binds to the target site) from binding to a target area. It will be appreciated by one of skill in the art that it is not necessary that the complementarity between a candidate chemical compound and a target site extend over all residues specified here in order to inhibit or promote binding of a ligand.

In general, the design of a chemical compound stereochemical complementarity possessing can accomplished by means of techniques that optimize, chemically or geometrically, the "fit" between a chemical compound and a target site. Such techniques are disclosed by, for example, Sheridan and Venkataraghavan, Acc. Chem Res., vol. 20, p. 322, 1987: Goodford, J. Med. Chem., vol. 27, p. 557, 1984; Beddell, Chem. Soc. Reviews, vol. 279, 1985; Hol, Angew. Chem., vol. 25, p. 767, 1986; and Verlinde and Hol, Structure, vol. 2, p. 577, 1994, each of which are incorporated by this reference herein in their entirety.

One embodiment of the present invention for structure based drug design comprises identifying a chemical compound

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that complements the shape of an FcR protein or a structure that is related to an FcR protein. Such method is referred to herein as a "geometric approach". In a geometric approach of the present invention, the number of internal degrees of freedom (and the corresponding local minima in the molecular conformation space) is reduced by considering only the geometric (hard-sphere) interactions of two rigid bodies, where one body (the active site) contains "pockets" or "grooves" that form binding sites for the second body (the complementing molecule, such as a ligand).

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The geometric approach is described by Kuntz et al., Mol. Biol., vol. 161, p. 269, 1982, J. incorporated by this reference herein in its entirety. algorithm for chemical compound design can be implemented using the software program DOCK Package, Version 1.0 (available from the Regents of the University of California). Pursuant to the Kuntz algorithm, the shape of the cavity or groove on the surface of a structure (e.g., FcyRIIa protein) at a binding site or interface is defined as a series of overlapping spheres of different radii. or more extant databases of crystallographic data (e.g., the Cambridge Structural Database System maintained by University Chemical Laboratory, Cambridge University, Lensfield Road, Cambridge CB2 1EW, U.K.) or the Protein Data Bank maintained by Brookhaven National Laboratory, is then searched for chemical compounds that approximate the shape thus defined.

Chemical compounds identified by the geometric approach can be modified to satisfy criteria associated with chemical complementarity, such as hydrogen bonding, ionic interactions or Van der Waals interactions.

Another embodiment of the present invention for structure based drug design comprises determining the interaction of chemical groups ("probes") with an active

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site at sample positions within and around a binding site or interface, resulting in an array of energy values from which three dimensional contour surfaces at selected energy levels can be generated. This method is referred to herein a "chemical-probe approach." The chemical-probe approach to the design of a chemical compound of the present invention is described by, for example, Goodford, J. Med. Chem., vol. 28, p. 849, 1985, which is incorporated by this reference herein in its entirety, appropriate software implemented using an package, including for example, GRID (available from Molecular Discovery Ltd., Oxford OX2 9LL, U.K.). The chemical prerequisites for a site-complementing molecule can be identified at the outset, by probing the active site of an FcyRIIa protein, for example, (as represented by the atomic coordinates shown in Table 1) with different chemical probes, e.g., water, a methyl group, an amine nitrogen, a carboxyl oxygen and/or a hydroxyl. Preferred sites for interaction between an active site and a probe are determined. Putative complementary chemical compounds can be generated using the resulting three dimensional pattern of such sites.

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A therapeutic composition of the present invention can comprise one or more therapeutic compounds of the present invention. A therapeutic composition can further comprise other compounds capable of reducing Iq-mediated responses or increasing a humoral immune response. For example, a therapeutic composition of the present invention useful for reducing tissue damage can also include compounds that block recruitment of inflammatory cells, such as by, for example, blocking complement fixation, extravasation, block binding of viral proteins to FcR, block opsinization or enhance normal and passive antibody immunity. therapeutic composition of the present invention useful for reducing Ig-mediated inflammation can include compounds

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that block recruitment of inflammatory cells and/or block signal transduction pathway which leads to the release of inflammatory mediators.

A therapeutic composition of the present invention useful for increasing a humoral response can also include compounds that increase antibody production against an antigen (i.e., adjuvants), including, but not limited to, cytokines, chemokines, and compounds that induce the production of cytokines and chemokines (e.g., granulocyte macrophage colony stimulating factor (GM-CSF), granulocyte colony stimulating factor (G-CSF), macrophage colony stimulating factor (M-CSF), colony stimulating factor erythropoietin (EPO), interleukin (IL-2), interleukin-3 (IL-3), interleukin 4 (IL-4), interleukin 5 interleukin 6 (IL-6), interleukin 7 (IL-7), (TL-5), interleukin 8 (IL-8), interleukin 10 (IL-10), interleukin 12 (IL-12), interferon gamma, interferon gamma inducing factor I (IGIF), transforming growth factor beta, RANTES (regulated upon activation, normal T cell expressed and presumably secreted), macrophage inflammatory proteins (e.g., MIP-1 alpha and MIP-1 beta), bacterial components (e.g., endotoxins, in particular superantigens, exotoxins cell wall components); aluminum-based salts: calcium-based salts; silica; polynucleotides; toxoids; serum proteins, viral coat proteins; block copolymer adjuvants (e.g., Hunter's Titermax™ adjuvant (Vaxcel™, Inc. Norcross, GA), Ribi adjuvants (Ribi ImmunoChem Research, Inc., Hamilton, MT); and saponins and their derivatives (e.g., Quil A (Superfos Biosector A/S, Denmark).

A therapeutic composition of the present invention can be used to treat disease in an animal by administering such composition to an animal in such a manner that desired therapeutic results are obtained. Preferred animals to treat include mammals, marsupials, reptiles and birds, with humans, companion animals, food animals, zoo animals and

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other economically relevant animals (e.g., race horses and animals valued for their coats, such as chinchillas and minks). More preferred animals to treat include humans, dogs, cats, horses, cattle, sheep, swine, chickens, ostriches, emus, turkeys, koalas and kangaroos. Particularly preferred animals to protect are humans, dogs and cats.

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A preferred therapeutic composition of the present invention also includes an excipient, an adjuvant and/or carrier. Suitable excipients include compounds that the animal to be treated can tolerate. Examples of such excipients include water, saline, Ringer's solution, dextrose solution, Hank's solution, and other aqueous physiologically balanced salt solutions. Nonaqueous vehicles, such as fixed oils, sesame oil, ethyl oleate, or triglycerides may also be used. Other useful formulations include suspensions containing viscosity enhancing agents, sodium carboxymethylcellulose, sorbitol, as dextran. Excipients can also contain minor amounts of additives, such as substances that enhance isotonicity and chemical stability. Examples of buffers include phosphate buffer, bicarbonate buffer and Tris buffer, while examples of preservatives include thimerosal, o-cresol, formalin and benzyl alcohol. Standard formulations can either be liquid injectables or solids which can be taken up in a suitable liquid as a suspension or solution for injection. Thus, in a non-liquid formulation, the excipient can comprise dextrose, human serum albumin, preservatives, etc., to which sterile water or saline can be added prior to administration.

In one embodiment of the present invention, a therapeutic composition can include a carrier. Carriers include compounds that increase the half-life of a therapeutic composition in the treated animal. Suitable carriers include, but are not limited to, polymeric

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controlled release vehicles, biodegradable implants, liposomes, bacteria, viruses, other cells, oils, esters, and glycols.

therapeutic administer protocols to Acceptable compositions of the present invention in an effective manner include individual dose size, number of doses, of mode administration, and dose frequency of Determination of such protocols can be administration. accomplished by those skilled in the art. Modes of administration can include, but are not limited to, subcutaneous, intradermal, intravenous, intranasal, oral, transdermal, intraocular and intramuscular routes.

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Another embodiment of the present invention are diagnostic compounds capable of detecting altered FcR protein on or isolated from cells obtained from patients having abnormal immunity or inflammation. Using the methods of structure based drug design described herein, diagnostic reagents that bind to FcR protein can be developed using the three dimensional structure of FcR Preferred diagnostic reagents of the present protein. invention include molecules capable of binding to the Ig binding site of an FcR protein capable of binding to Ig and molecules capable of binding to circulating FcR protein obtained from patients with inflammation. Preferred diagnostic reagents include molecules that are immunogenic or can be chemically coupled to detectable compounds, such as radioisotopes, enzymes, dyes or biotin.

In a preferred embodiment, a therapeutic compound or diagnostic compound of the present invention comprises a protein engineered by recombinant DNA methods.

TABLE 1

REMARK Latest coordinates of the Fc Gamma Receptor IIa structure REMARK Written by O version 5.10.1 REMARK Wed May 20 10:23:51 1998 35 28.172 90.00 90.00 90.00 79.221 100.866 CRYST1 1.000000 0.000000 0.000000 0.000000 1.000000 0.000000 0.00000 ORIGX1 0.00000 ORIGX2 0.00000 0.000000 0.000000 1.000000 ORIGX3 0.012623 0.000000 0.000000 0.00000 40 SCALE1

	SCALE2 SCALE3			00000	0.009914	0.0000		0.0000		
	ATOM	1	CB	ALA	1	36.645				ϵ
	ATOM	2	c	ALA	ī	36.199				6
5	ATOM	3	ō	ALA	ī	36.801		-1.569		8
	ATOM	4	N	ALA	ī	34.367		-3.997		7
	ATOM	5	CA	ALA	1	35.829		-3.724	1.00 43.68	Ė
	ATOM	6	N	PRO	2	35.903		-1.817	1.00 40.54	7
	ATOM	7	CD	PRO	2	35.149	70.546	-2.533	1.00 38.91	6
10	ATOM	8	CA	PRO	2	36.172		-0.425	1.00 38.61	6
	ATOM	9	CB	PRO	2	35.765		-0.322	1.00 39.86	6
	MOTA	10	CG	PRO	2	34.790		-1.426	1.00 41.36	6
	ATOM	11	С	PRO	2	35.294		0.434	1.00 36.70	6
15	ATOM	12	0	PRO	2	34.188	68.654	-0.042	1.00 32.46	8
10	ATOM ATOM	13 14	N CD	PRO PRO	3 3	35.789		1.579	1.00 33.82	7
	ATOM	15	CA	PRO	3	37.120 35.069	68.857 67.637	2.110 2.491	1.00 35.16	6
	ATOM	16	CB	PRO	3	35.872	67.639	3.799	1.00 38.25 1.00 37.39	6 6
	ATOM	17	CG	PRO	3	37.180	68.267	3.486	1.00 37.33	6
20	ATOM	18	c	PRO	3	33.653	68.136	2.790	1.00 37.41	6
	ATOM	19	0	PRO	3	33.393	69.335	2.683	1.00 34.39	8
	ATOM	20	N	LYS	4	32.763	67.212	3.173	1.00 37.04	7
	ATOM	21	CA	LYS	4	31.3 9 9	67.678	3.424	1.00 34.97	6
	ATOM	22	CB	LYS	4	30.318	66.664	3.122	1.00 43.98	6
25	MOTA	23	CG	LYS	4	30.564	65.191	3.278	1.00 47.64	6
	MOTA	24	CD	LYS	4	29.775	64.349	2.292	1.00 52.03	6
	MOTA	25	CE	LYS	4	28.317	64.743	2.137	1.00 57.56	6
	ATOM	26	NZ	LYS	4	27.724	64.253	0.855	1.00 56.40	7
20	ATOM	27	С	LYS	4	31.243	68.234	4.825	1.00 31.44	6
30	ATOM	28	0	LYS	4	31.846	67.769	5.784	1.00 29.91	8
	ATOM	29	N	ALA	5	30.416	69.280	4.908	1.00 28.75	7
	ATOM ATOM	30 31	CA CB	ALA ALA	5 5	30.039 29.155	69.813	6.218	1.00 27.21	6
	ATOM	32	C	ALA	5	29.133	71.032 68.683	6.110 6.923	1.00 21.94 1.00 26.42	6
35	ATOM	33	õ	ALA	5	28.760	67.794	6.222	1.00 26.42	6 8
	ATOM	34	N	VAL	6	29.231	68.674	8.241	1.00 24.91	7
	ATOM	35	CA	VAL	6	28.515	67.632	8.985	1.00 26.95	6
	ATOM	36	CB	VAL	6	29.490	66.738	9.770	1.00 29.36	6
	ATOM	37	CG1	VAL	6	28.779	65.726	10.676	1.00 29.86	6
40	ATOM	38	CG2	VAL	6	30.434	66.024	8.801	1.00 26.74	6
	ATOM	39	C	VAL	6	27.503	68.253	9.942	1.00 28.93	6
	ATOM	40	0	VAL	6	27.846	68.994	10.866	1.00 31.46	8
	ATOM	41	N	LEU	7	26.233	67.929	9.758	1.00 30.08	7
ΛE	ATOM	42	CA	LEU	7	25.105	68.383	10.546	1.00 29.33	6
45	ATOM	43	CB	LEU	7	23.839	68.346	9.657	1.00 33.18	6
	MOTA MOTA	44 45	CG CD1	LEU LEU	7 7	22.828	69.458	9.960	1.00 34.94	6
	ATOM	46		LEU	7	22.082 21.887	69.876 69.002	8.721 11.069	1.00 27.55 1.00 32.30	6
	ATOM	47	C	LEU	ź	24.816	67.565	11.794	1.00 32.30	6 6
50	ATOM	48	ŏ	LEU	ż	24.653	66.351	11.800	1.00 29.37	8
	ATOM	49	N	LYS	8	24.768	68.242	12.930	1.00 28.04	7
	ATOM	50	CA	LYS	8	24.568	67.692	14.257	1.00 25.12	6
	ATOM	51	CB	LYS	8	25.738	68.179	15.132	1.00 33.32	6
	MOTA	52	CG	LYS	8	25.777	67.611	16.532	1.00 39.37	6
55	ATOM	53	CD	LYS	8	25.967	68.598	17.652	1.00 43.84	6
	MOTA	54	CE	LYS	8	27.12 9	69.561	17.487	1.00 47.78	6
	ATOM	55	NZ	LYS	8	27.525	70.175	18.793	1.00 48.98	7
	ATOM	56	С	LYS	8	23.233	68.192	14.797	1.00 24.53	6
C0	ATOM	57	0	LYS	8	22.934	69.384	14.739	1.00 25.35	8
60	ATOM	58	N	LEU	9	22.423	67.310	15.333	1.00 24.78	7
	MOTA	59	CA	LEU	9	21.080	67.553	15.843	1.00 22.07	6
	MOTA	60	CB	LEU	9	20.189	66.483	15.190	1.00 20.04	6
	ATOM	61	CG CD1	LEU	9	18.725	66.363	15.596	1.00 20.57	6
65	ATOM ATOM	62 63	CD1		9 9	17.980	67.624	15.214	1.00 19.57	6
00	ATOM ATOM	64	CD2 C	LEU	9	18.084	65.137	14.903	1.00 23.44	6
	ATOM	65	0	LEU	9	21.019	67.415 66.393	17.346 17.869	1.00 21.01	6
	ATOM	66	N	GLU	10	20.583	68.410	18.118	1.00 22.38 1.00 22.53	8 7
	ATOM	67	CA	GLU	10	20.480	68.285	19.567	1.00 22.33	6
70	ATOM	68	СВ	GLU	10	21.523	69.182	20.270	1.00 27.36	6
	ATOM	69	CGA		10	22.971	68.778	20.090	0.50 28.21	6

	ATON ATON ATON	71 CDA GLU	10	22.946 68.657 20.195 0.50 38.29 6 24.047 69.789 20.422 0.50 28.55 6
5	ATOM ATOM ATOM	73 OE1 GLU 74 OE1 GLU	10 10	23.100 67.202 20.587 0.50 43.48 6 25.131 69.365 20.907 0.50 26.56 8 22.443 66.771 21.565 0.50 47.24 8
	ATOM ATOM ATOM	76 OE2 GLU 77 C GLU	10 10	23.888 71.008 20.186 0.50 22.10 8 23.871 66.486 19.908 0.50 46.42 8 19.096 68.728 20.008 1.00 19.76 6
10	ATOM ATOM ATOM	79 N PRO 80 CD PRO	11 11 11	18.701 69.842 19.613 1.00 18.00 8 18.423 67.995 20.888 1.00 19.07 7 17.058 68.340 21.390 1.00 18.71 6 18.834 66.662 21 319 1.00 18.74 6
15	MOTA MOTA MOTA		11 11 11	17.807 66.272 22.365 1.00 17.38 6 16.560 67.000 21.944 1.00 18.86 6
	ATOM ATOM ATOM	85 O PRO 86 N PRO 87 CD PRO	11 12 12	18.310 66.212 19.051 1.00 16.22 8 19.232 64.517 20.155 1.00 19.94 7
20	MOTA MOTA MOTA	88 CA PRO 89 CB PRO 90 CG PRO	12 12 12	19.409 63.700 18.976 1.00 20.68 6 20.455 62.656 19.397 1.00 19.82 6 20.292 62.567 20.872 1.00 23.59 6
25	MOTA MOTA MOTA	91 C PRO 92 O PRO 93 N TRP 94 CA TRP	12 12 13	18.179 63.061 18.395 1.00 18.70 6 18.268 62.475 17.318 1.00 19.85 8 17.039 63.169 19.059 1.00 15.64 7
	ATOM ATOM ATOM	95 CB TRP 96 CG TRP 97 CD2 TRP	13 13 13 13	15.815 62.568 18.561 1.00 17.91 6 14.688 62.840 19.562 1.00 14.32 6 15.124 62.749 21.006 1.00 16.77 6
30	ATOM ATOM ATOM	98 CE2 TRP 99 CE3 TRP 100 CD1 TRP	13 13 13	15.899 62.005 23.032 1.00 16.87 6 15.867 60.279 21.350 1.00 18.03 6
35	ATOM ATOM ATOM ATOM	101 NE1 TRP 102 CZ2 TRP 103 CZ3 TRP	13 13 13	15.106 63.769 21.916 1.00 18.97 6 15.589 63.343 23.137 1.00 11.16 7 16.405 61.124 23.973 1.00 15.92 6 16.358 59.409 22.301 1.00 10.59 6
55	MOTA MOTA MOTA	104 CH2 TRP 105 C TRP 106 O TRP 107 N ILE	13 13 13	16.645 59.825 23.611 1.00 17.87 6 15.421 63.033 17.163 1.00 19.47 6 15.283 64.238 16.908 1.00 17.22 8
40	ATOM ATOM ATOM	108 CA ILE 109 CB ILE 110 CG2 ILE	14 14 14 14	15.101 62.078 16.275 1.00 16.57 7 14.666 62.441 14.936 1.00 18.93 6 15.185 61.523 13.816 1.00 16.07 6 16.720 61.521 13.840 1.00 16.61 6
4.E	MOTA ATOM ATOM	111 CG1 ILE 112 CD1 ILE 113 C ILE	14 14 14	14.582 60.119 13.972 1.00 21.35 6 15.045 59.150 12.896 1.00 26.28 6
45	ATOM ATOM ATOM	114 O ILE 115 N ASN 116 CA ASN	14 15 15	13.144 62.549 14.825 1.00 20.48 6 12.652 63.048 13.817 1.00 19.41 8 12.403 62.087 15.836 1.00 19.46 7 10.935 62.270 15.778 1.00 18.11 6
50	ATOM ATOM ATOM ATOM	117 CB ASN 118 CG ASN 119 OD1 ASN 120 ND2 ASN	15 15 15 15	10.161 60.962 15.731 1.00 13.53 6 10.591 59.946 16.762 1.00 19.11 6 11.728 59.959 17.227 1.00 13.35 8
	ATOM ATOM ATOM	121 C ASN 122 O ASN 123 N VAL	15 15 15 16	9.688 59.033 17.142 1.00 10.11 7 10.632 63.124 17.005 1.00 17.54 6 11.016 62.735 18.111 1.00 15.32 8 10.122 64.331 16.805 1.00 16.86 7
55	ATOM ATOM ATOM	124 CA VAL 125 CB VAL 126 CG1 VAL	16 16 16	10.122 64.331 16.805 1.00 16.86 7 9.871 65.273 17.893 1.00 15.77 6 10.761 66.534 17.748 1.00 16.54 6 12.251 66.141 17.733 1.00 13.42 6
60	ATOM ATOM ATOM ATOM ATOM	127 CG2 VAL 128 C VAL 129 O VAL 130 N LEU 131 CA LEU	16 16 16 17 17	10.490 67.345 16.491 1.00 18.04 6 8.420 65.708 17.921 1.00 19.01 6 7.618 65.381 17.010 1.00 17.12 8 8.022 66.422 18.964 1.00 17.68 7
65	ATOM ATOM ATOM ATOM	132 CB LEU 133 CG LEU 134 CD1 LEU 135 CD2 LEU	17 17 17 17	6.162 66.726 20.522 1.00 20.26 6 5.873 65.251 20.823 1.00 23.07 6 5.447 65.013 22.253 1.00 17.70 6
70	ATOM ATOM ATOM ATOM	136 C LEU 137 O LEU 138 N GLN 139 CA GLN 140 CB GLN	17 / 17 18 18 18	4.832 64.714 19.855 1.00 26.74 6 6.563 68.439 18.732 1.00 16.37 6 7.518 69.187 18.961 1.00 18.24 8 5.424 68.931 18.227 1.00 18.55 7 5.237 70.370 18.032 1.00 19.13 6 3.790 70.721 17.696 1.00 31.65 6

	2001	141 CG GLN	18	3.510	71.249	16.314	1.00 37.32	6
	ATOM ATOM	141 CG GLN 142 CD GLN	18	2.120	70.902	15.800	1.00 36.92	6
	ATOM	143 OE1 GLN	18	1.953	70.032	14.943	1.00 30.97	8
	ATOM	144 NE2 GLN	18	1.135	71.618	16.333	1.00 31.73	7
5	ATOM	145 C GLN	18	5.561	71.077	19.348	1.00 19.43 1.00 18.10	6 8
	MOTA	146 O GLN	18	5.194	70.568	20.413	1.00 19.68	7
	MOTA	147 N GLU	19	6.317	72.164 73.045	20.293	1.00 18.88	6
	MOTA	148 CA GLU	19 19	6.727 5.597	73.341	21.293	1.00 27.39	6
7.0	MOTA	149 CB GLU 150 CG GLU	19	4.649	74.418	20.714	1.00 30.12	6
10	MOTA	150 CG GLU 151 CD GLU	19	3.558	74.699	21.720	1.00 41.87	6
	MOTA MOTA	152 OE1 GLU	19	3.857	75.330	22.758	1.00 48.83	8
	ATOM	153 OE2 GLU	19	2.421	74.272	21.464	1.00 46.61	8
	ATOM	154 C GLU	19	8.004	72.622	20.998	1.00 21.46 1.00 26.39	6 8
15	MOTA	155 O GLU	19	8.496	73.405	21.815 20.619	1.00 20.33	7
	MOTA	156 N ASP	20	8.606 9.898	71.506 71.094	21.114	1.00 20.76	6
	ATOM	157 CA ASP 158 CB ASP	20 20	10.285	69.649	20.726	1.00 13.47	6
	MOTA	158 CB ASP 159 CG ASP	20	9.587	68.578	21.526	1.00 13.93	6
20	MOTA MOTA	160 OD1 ASP	20	8.873	68.805	22.534	1.00 17.57	8
20	ATOM	161 OD2 ASP	20	9.723	67.405	21.104	1.00 13.79	8
	ATOM	162 C ASP	20	11.002	71.950	20.451	1.00 19.58	6
	ATOM	163 O ASP	20	10.913	72.219	19.262	1.00 17.49	8 7
	ATOM	164 N SER	21	12.071	72.198	21.174	1.00 17.22 1.00 17.62	6
25	MOTA	165 CA SER	21	13.233	72.929 73.525	20.659 21. 844	0.50 17.49	6
	ATOM	166 CBA SER	21 21	14.011 13.981	73.556	21.846	0.50 13.14	6
	MOTA	167 CBB SER 168 OGA SER	21	14.900	74.516	21.355	0.50 22.95	8
	ATOM ATOM	169 OGB SER	21	13.175	74.579	22.416	0.50 6.85	8
30	ATOM	170 C SER	21	14.181	72.038	19.873	1.00 18.61	6
50	ATOM	171 O SER	21	14.424	70.884	20.265	1.00 21.41	8
	MOTA	172 N VAL	22	14.638	72.512	18.721	1.00 15.80 1.00 17.93	7 6
	ATOM	173 CA VAL	22	15.585	71.733 71.234	17.910 16.560	1.00 17.33	6
	ATOM	174 CB VAL	22	15.052 16.093	70.401	15.804	1.00 17.77	6
35	MOTA	175 CG1 VAL 176 CG2 VAL	22 22	13.858	70.300	16.679	1.00 17.26	6
	MOTA MOTA	176 CG2 VAL 177 C VAL	22	16.822	72.609	17.665	1.00 19.20	6
	ATOM	178 O VAL	22	16.633	73.769	17.291	1.00 18.52	8
	ATOM	179 N THR	23	18.021	72.107	17.917	1.00 16.32	7
40	ATOM	180 CA THR	23	19.249	72.823	17.648	1.00 19.99 1.00 22.97	6 6
	MOTA	181 CB THR	23	20.080	73.128 73.749	18.911 19.850	1.00 22.37	8
	ATOM	182 OG1 THR	23 2 3	19.192 21.241	74.057	18.614	1.00 16.78	6
	MOTA	183 CG2 THR 184 C THR	23	20.098	72.016	16.658	1.00 24.68	6
45	MOTA MOTA	185 O THR	23	20.509	70.880	16.897	1.00 22.59	8
40	ATOM	186 N LEU	24	20.257	72.618	15.467	1.00 23.73	7
	ATOM	187 CA LEU	24	21.081	72.051	14.423	1.00 23.11	6 6
	ATOM	188 CB LEU	24	20.427	72.206	13.046	1.00 20.25 1.00 23.95	6
	MOTA	189 CG LEU	24	19.053	71.480	12.959 11.681	1.00 20.78	6
50	MOTA	190 CD1 LEU	24	18.324 19.251	71.856 69.985	13.049	1.00 22.74	6
	MOTA	191 CD2 LEU	24 24	22.444	72.763		1.00 25.87	6
	ATOM	192 C LEU 193 O LEU	24	22.470	74.008	14.537	1.00 24.57	8
	ATOM ATOM	194 N THR	25	23.520	71.980	14.367	1.00 20.22	7
55	ATOM	195 CA THR	25	24.847	72.600	14.336	1.00 23.21	6
00	ATOM	196 CB THR	25	25.656	72.265	15.597	1.00 27.69	6
	MOTA	197 OG1 THR	25	24.945	72.730	16.755	1.00 26.30 1.00 28.49	8 6
	ATOM	198 CG2 THR	25	27.041	72.925 72.166	15.590 13.075	1.00 22.31	6
	ATOM	199 C THR	25 25	25.604 25.706	70.951	12.819	1.00 23.86	8
6 0	ATOM	200 O THR 201 N CYS	26	26.092	73.134	12.307	1.00 18.68	7
	MOTA MOTA	201 N CYS 202 CA CYS	26	26.832		11.075	1.00 23.20	6
	ATOM	203 C CYS	26	28.345	72.910	11.346	1.00 23.06	6
	ATOM	204 O CYS	26	28.957		11.556	1.00 23.76	8
65	MOTA	205 CB CYS	26	26.509		9.958	1.00 17.92 1.00 22.25	6 16
	ATOM	206 SG CYS	26	27.138	73.358	8.311 11.355	1.00 22.25	7
	MOTA	207 N GLN	27	28.929 30.332		11.658	1.00 23.30	6
	MOTA	208 CA GLN 209 CB GLN	27 27	30.543		12.464	1.00 29.78	6
70	MOTA MOTA	209 CB GLN 210 CG GLN	27	29.623		13.672	1.00 31.50	6
70	ATOM	211 CD GLN	27	29.927		14.518	1.00 33.01	6

	MOTA	212	OE1	GLN	27	30.322	67.774	14.032	1.00 38.67	8
	MOTA	213	NE2	GLN	27	29.792	68.895	15.834	1.00 36.36	7
	MOTA	214	C	GLN	27	31.169	71.417	10.377	1.00 26.33	6
	ATOM	215	0	GLN	27	30.764	70.856	9.347	1.00 23.15	8
5	MOTA	216	N	GLY	28	32.363	72.019	10.438	1.00 27.69	7
	MOTA	217	CA	GLY	28	33.289	72.019	9.313	1.00 28.02	6
	MOTA	218	С	GLY	28	34.022	73.360	9.215	1.00 29.41	6
	MOTA	219	0	GLY	28	33.639	74.335	9.862	1.00 28.46	8
	MOTA	220	N	ALA	29	35.062	73.421	8.389	1.00 27.48	7
10	MOTA	221	CA	ALA	29	35.824	74.640	8.210	1.00 27.39	6
	MOTA	222	CB	ALA	29	36.979	74.353	7.239	1.00 25.91	6
	MOTA	223	С	ALA	29	34.959	75.730	7.574	1.00 28.27	6
	MOTA	224	0	ALA	29	34.315	75.415	6.561	1.00 26.07 1.00 23.97	8 7
3 C	MOTA	225	N	ARG	30	35.060	76.951	8.064 7.490	1.00 23.37	6
15	MOTA	226	CA	ARG	30	34.303 33.571	78.055 78.823	8.601	1.00 30.34	6
	MOTA	227	CB	ARG ARG	30 30	32.574	78.090	9.460	1.00 34.05	6
	ATOM	228 229	CD	ARG	30	32.365	78.880	10.761	1.00 33.86	6
	ATOM ATOM	230	NE	ARG	30	32.407	77.902	11.836	1.00 38.60	7
20	ATOM	231	CZ	ARG	30	32.487	78.082	13.126	1.00 38.08	6
20	ATOM	232		ARG	30	32.567	79.298	13.635	1.00 36.51	7
	ATOM	233	NH2	ARG	30	32.467	76.990	13.879	1.00 46.13	7
	ATOM	234	С	ARG	30	35.194	79.148	6.880	1.00 26.70	6
	ATOM	235	0	ARG	30	36.399	79.142	7.075	1.00 29.22	8
25	ATOM	236	N	SER	31	34.573	80.129	6.246	1.00 26.85	7
	ATOM	237	CA	SER	31	35.315	81.284	5.738	1.00 26.56	6
	ATOM	238	CB	SER	31	34.682	81.846	4.476	1.00 25.03	6
	MOTA	239	OG	SER	31	34.562	80.875	3.477	1.00 27.59	8
	MOTA	240	С	SER	31	35.273	82.321	6.861	1.00 26.58	6
30	MOTA	241	0	SER	31	34.396	82.246	7.739	1.00 23.91	8
	ATOM	242	N	PRO	32	36.163	83.308	6.839	1.00 23.48	7
	MOTA	243	CD	PRO	32	37.224	83.483	5.842	1.00 22.70	6
	MOTA	244	CA	PRO	32	36.176	84.350	7.861	1.00 24.75	6
2.5	ATOM	245	CB	PRO	32	37.621	84.830	7.805	1.00 24.34	6 6
35	MOTA	246	CG	PRO	32	38.095	84.571 85.449	6.414 7.549	1.00 23.77 1.00 29.23	6
	MOTA	247	C	PRO	32 32	35.172 35.472	86.609	7.223	1.00 28.28	8
	MOTA	248	0	PRO	32	33.913	85.121	7.709	1.00 29.77	7
	MOTA	249 250	n Ca	GLU GLU	33	32.725	85.896	7.417	1.00 33.37	6
40	ATOM ATOM	251		GLU	33	32.177	85.426	6.073	0.50 35.18	6
40	ATOM	252		GLU	33	32.123	85.457	6.084	0.50 31.98	6
	ATOM	253		GLU	33	30.795	84.829	5.952	0.50 39.40	6
	ATOM	254		GLU	33	31.776	83.990	5.954	0.50 34.05	6
	ATOM	255		GLU	33	30.394	84.525	4.521	0.50 46.48	6
45	MOTA	256	CDB	GLU	33	31.601	83.533	4.517	0.50 34.67	6
	MOTA	257	OE1	GLU	33	29.268	84.856	4.076	0.50 49.23	8
	MOTA	258	OE1	GLU	33	32.194	84.168	3.619	0.50 32.81	8
	MOTA	259	OE2	GLU	33	31.232	83.952	3.788	0.50 47.50	8
	MOTA	260	OE2	GLU	33	30.877	82.542	4.275	0.50 24.64	8
50	ATOM	261	С	GLU	33	31.683	85.689	8.519	1.00 32.61	6
	MOTA	262	0	GLU	33	31.612	84.600	9.085	1.00 28.72	8 7
	ATOM	263	N	SER	34	30.844	86.682	8.743	1.00 32.15	6
	MOTA	264	CA	SER	34	29.804	86.591	9.764	1.00 32.72	6
	ATOM	265	CB	SER	34	29.277	88.013	10.037 11.093	1.00 34.26 1.00 45.88	8
55	ATOM	266	OG	SER	34	28.320	87.931	9.332	1.00 30.93	6
	ATOM	267	c	SER	34	28.668 28.156	85.674 84.883	10.124	1.00 28.87	8
	ATOM	268	0	SER	34 35	28.222	85.773	8.082	1.00 28.02	7
	ATOM	269	N	ASP ASP	35	27.167	84.858	7.599	1.00 28.62	6
60	ATOM ATOM	270 271	CA CB	ASP	35	26.292	85.538	6.585	1.00 29.65	6
00	ATOM	272	CG	ASP	35	25.357	86.639	7.057	1.00 37.43	6
	ATOM	273		ASP	35	25.027	86.769	8.258	1.00 33.53	8
	ATOM	274		ASP	35	24.902	87.396	6.154	1.00 36.01	8
	ATOM	275	C	ASP	35	27.882	83.643	6.973	1.00 27.08	6
65	ATOM	276	ō	ASP	35	27.997	83.566	5.756	1.00 28.07	8
	MOTA	277	N	SER	36	28.461	82.748	7.774	1.00 25.55	7
	ATOM	278	CA.	SER	36	29.282	81.680	7.225	1.00 27.45	6
	ATOM	279	CB	SER	36	30.440	81.431	8.213	1.00 34.87	6
	ATOM	280	OG	SER	36	29.973	80.802	9.405	1.00 39.51	8
70	ATOM	281	С	SER	36	28.558	80.382	6.890	1.00 27.14	6
	MOTA	282	0	SER	36	29.143	79.421	6.363	1.00 25.67	8

5	ATOM ATOM ATOM ATOM ATOM ATOM	284 CA ILE 285 CB ILE	37 37 37	27.293 80.223 7.231 1.00 24.64 7 26.580 78.973 6.977 1.00 24.33 6 26.164 78.307 8.309 1.00 30.71 6 25.561 76.931 8.032 1.00 26.94 6 27.333 78.221 9.308 1.00 21.66 6 28.443 77.278 8.867 1.00 27.66 6
10	ATOM ATOM ATOM ATOM ATOM ATOM	289 C ILE 290 O ILE 291 N GLN 292 CA GLN 293 CB GLN 294 CG GLN	37 37 38 38 38 38	25.336 79.159 6.128 1.00 24.08 6 24.515 80.033 6.390 1.00 23.50 8 25.122 78.314 5.127 1.00 24.52 7 23.862 78.296 4.399 1.00 23.13 6 24.016 78.068 2.905 1.00 29.28 6 24.458 79.296 2.123 1.00 29.86 6
15	ATOM ATOM ATOM ATOM	295 CD GLN 296 OE1 GLN 297 NE2 GLN 298 C GLN 299 O GLN	38 38 38 38 38	24.692 78.965 0.661 1.00 33.48 6 25.540 78.122 0.323 1.00 28.34 8 23.922 79.668 -0.177 1.00 38.54 7 23.048 77.128 4.985 1.00 23.81 6 23.598 76.022 5.087 1.00 22.62 8
20	ATOM ATOM ATOM ATOM ATOM	300 N TRP 301 CA TRP 302 CB TRP 303 CG TRP 304 CD2 TRP	39 39 39 39	21.807 77.386 5.371 1.00 21.43 7 20.987 76.304 5.905 1.00 21.73 6 20.345 76.633 7.257 1.00 21.01 6 21.264 76.633 8.430 1.00 17.58 6 21.721 75.523 9.212 1.00 17.00 6
25	ATOM ATOM ATOM ATOM ATOM	305 CE2 TRP 306 CE3 TRP 307 CD1 TRP 308 NE1 TRP 309 CZ2 TRP	39 39 39 39 39	22.569 76.033 10.220 1.00 16.71 6 21.495 74.147 9.158 1.00 21.47 6 21.844 77.750 8.974 1.00 19.92 6 22.626 77.400 10.061 1.00 22.18 7 23.218 75.220 11.152 1.00 18.29 6
30	ATOM ATOM ATOM ATOM MOTA	310 CZ3 TRP 311 CH2 TRP 312 C TRP 313 O TRP 314 N PHE	39 39 39 39 40	22.109 73.329 10.091 1.00 21.62 6 22.960 73.874 11.064 1.00 20.15 6 19.890 75.993 4.898 1.00 22.76 6 19.407 76.925 4.238 1.00 23.42 8
35	ATOM ATOM ATOM ATOM ATOM	315 CA PHE 316 CB PHE 317 CG PHE 318 CD1 PHE 319 CD2 PHE	40 40 40 40 40	18.512 74.389 3.754 1.00 26.86 6 19.121 73.722 2.513 1.00 24.16 6 20.225 74.429 1.788 1.00 23.96 6 21.551 74.280 2.189 1.00 23.61 6
40	ATOM ATOM ATOM ATOM ATOM	320 CE1 PHE 321 CE2 PHE 322 CZ PHE 323 C PHE 324 O PHE	40 40 40 40 40	22.564 74.919 1.504 1.00 20.83 6 20.967 75.880 0.020 1.00 21.69 6 22.267 75.740 0.432 1.00 21.86 6 17.466 73.435 4.349 1.00 23.51 6
45	ATOM ATOM ATOM ATOM ATOM	325 N HIS 326 CA HIS 327 CB HIS 328 CG HIS	41 41 41 41	17.838 72.588 5.151 1.00 21.94 8 16.232 73.575 3.905 1.00 21.59 7 15.107 72.771 4.366 1.00 24.07 6 14.032 73.572 5.099 1.00 18.72 6 12.864 72.727 5.548 1.00 23.41 6
50	ATOM ATOM ATOM ATOM	329 CD2 HIS 330 ND1 HIS 331 CE1 HIS 332 NE2 HIS 333 C HIS	41 41 41 41 41	12.794 71.415 5.899 1.00 21.85 6 11.588 73.218 5.709 1.00 21.97 7 10.789 72.259 6.135 1.00 22.79 6 11.504 71.161 6.268 1.00 21.87 7 14.455 72.163 3.115 1.00 21.83 6
55	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	334 O HIS 335 N ASN 336 CA ASN 337 CB ASN 338 CG ASN 339 OD1 ASN 340 ND2 ASN	41 42 42 42 42 42	13.972 72.919 2.282 1.00 21.37 8 14.576 70.847 2.959 1.00 22.08 7 14.077 70.196 1.726 1.00 20.46 6 12.562 70.322 1.722 1.00 18.21 6 11.925 69.397 2.761 1.00 22.74 6 12.473 68.343 3.087 1.00 24.40 8
60	ATOM ATOM ATOM ATOM	341 C ASN 342 O ASN 343 N GLY 344 CA GLY	42 42 42 43 43	10.804 69.804 3.341 1.00 18.43 7 14.733 70.811 0.488 1.00 21.32 6 14.085 71.047 -0.533 1.00 20.13 8 16.002 71.220 0.568 1.00 20.53 7 16.767 71.861 -0.480 1.00 20.83 6
65	ATOM ATOM ATOM ATOM ATOM	345 C GLY 346 O GLY 347 N ASN 348 CA ASN 349 CB ASN	43 43 44 44 44	16.586 73.360 -0.661 1.00 24.51 6 17.209 73.987 -1.550 1.00 25.30 8 15.633 73.970 0.051 1.00 21.27 7 15.391 75.393 -0.112 1.00 20.46 6
70	ATOM ATOM ATOM ATOM	350 CG ASN 351 OD1 ASN 352 ND2 ASN 353 C ASN	44 44 44 44	13.903 /5.734 0.000 1.00 23.82 6 13.049 74.834 -0.891 1.00 22.26 6 12.148 74.144 -0.409 1.00 25.47 8 13.382 74.787 -2.171 1.00 21.59 7 16.208 76.143 0.937 1.00 19.78 6

									4 00 00 07	0
	ATOM	354	0	ASN	44		75.778	2.107	1.00 22.07	8 7
	MOTA	355	N	LEU	45		77.188	0.523 1.459	1.00 22.22	6
	MOTA	356	CA	LEU	45	17.730	77.962 79.141	0.715	1.00 28.15	6
_	ATOM	357	CB	LEU	45	18.391 19.159	80.171	1.538	1.00 29.14	6
5	ATOM	358	CG CD1	LEU LEU	45 45	20.479	79.571	2.002	1.00 25.07	6
	MOTA	359 3 6 0		LEU	45	19.452	81.466	0.775	1.00 28.51	6
	ATOM ATOM	361	C	LEU	45	16.825	78.559	2.525	1.00 22.27	6
	ATOM	362	ō	LEU	45	15.748	78.997	2.118	1.00 20.13	8 7
10	ATOM	363	N	ILE	46	17.263	78.604	3.766 4.835	1.00 20.11 1.00 24.64	6
_	MOTA	364	CA	ILE	46	16.539 16.657	79.322 78.508	6.132	1.00 22.24	6
	MOTA	365	CB	ILE	46 46	16.007	79.134	7.358	1.00 21.33	6
	MOTA	366		ILE	46	16.111	77.072	5.945	1.00 20.74	6
15	MOTA MOTA	367 368		ILE	46	16.664	76.147	7.024	1.00 20.48	6
13	ATOM	369	c	ILE	46	17.351	80.625	5.006	1.00 25.53	6
	MOTA	370	0	ILE	46	18.419	80.600	5.624	1.00 22.91 1.00 30.56	8 7
	ATOM	371	N	PRO	47	16.937	81.747	4.444 3.620	1.00 30.30	6
	MOTA	372	CD	PRO	47	15.704	81.884 82.968	4.434	1.00 30.93	6
20	ATOM	373	CA	PRO	47	17.731 17.030	83.836	3.363	1.00 31.28	6
	MOTA	374	CB	PRO PRO	47 47	15.610	83.400	3.441	1.00 32.54	6
	MOTA	375 376	CG C	PRO	47	17.888	83.762	5.706	1.00 28.32	6
	ATOM ATOM	377	Ö	PRO	47	18.733	84.670	5.747	1.00 29.24	8
25	ATOM	378	N	THR	48	17.092	83.513	6.730	1.00 26.79	7 6
20	MOTA	379	CA	THR	48	17.135	84.298	7.971	1.00 26.97 1.00 31.78	6
	ATOM	380	CB	THR	48	15.698	84.323 82.958	8.532 8.520	1.00 31.45	8
	MOTA	381		THR	48 48	15.241 14.798	85.150	7.605	1.00 27.40	6
20	MOTA	382	CG2	THR	48	18.075	83.757	9.021	1.00 26.31	6
30	MOTA MOTA	383 384	c o	THR	48	18.206	84.334	10.113	1.00 28.00	8
	ATOM	385	N	HIS	49	18.698	82.602	8.772	1.00 24.44	7
	ATOM	386	CA.	HIS	49	19.612	81.942	9.707	1.00 24.19 1.00 25.11	6 6
	ATOM	387	CB	HIS	49	18.953	80.610	10.174	1.00 23.11	6
35	MOTA	388	CG	HIS	49	17.722 16.430	80.939 81.109	10.624	1.00 27.86	6
	ATOM	389		HIS	49 49	17.809	81.225	12.306	1.00 29.80	7
	MOTA	390 391		HIS	49	16.595	81.526	12.762	1.00 28.91	6
	ATOM ATOM	392		HIS	49	15.748	81.474	11.761	1.00 25.35	7
40	ATOM	393	c	HIS	49	20.923	81.588	9.041	1.00 23.08 1.00 20.57	6 8
	ATOM	394	0	HIS	49	20.942	80.805	8.075 9.497	1.00 25.11	7
	MOTA	395	N	THR	50	22.038 23.321	82.162 81.974	8.807	1.00 22.98	6
	ATOM	396	CA	THR	50 50	23.732	83.314	8.137	1.00 23.01	6
ΛC	ATOM	397 398	CB	THR L THR	50	23.843	84.252	9.231	1.00 18.66	8
45	MOTA MOTA	399		THR	50	22.757	83.817	7.101	1.00 19.07	6
	ATOM	400	c c	THR	50	24.460	81.645	9.766	1.00 24.61	6
	ATOM	401	ō	THR	50	25.640	81.772	9.393	1.00 26.17 1.00 24.52	8 7
	ATOM	402	N	GLN	51	24.126	81.274	10.985 11.995	1.00 24.32	6
50	ATOM	403		GLN	51	25.132	80.979 81.505	13.378	1.00 28.63	6
	MOTA	404		GLN	51 51	24.708 24.438	83.014	13.378	1.00 32.81	6
	MOTA	405 406		GLN GLN	51	25.677	83.810	12.995	1.00 38.53	6
	ATOM ATOM	407		1 GLN	51	26.606	83.952	13.802	1.00 37.60	8
5 5	MOTA	408		2 GLN	51	25.724	84.331	11.765	1.00 32.79	7 6
33	ATOM	409		GLN	51	25.411	79.487	12.101	1.00 26.69 1.00 26.27	8
	ATOM	410	0	GLN	51	24.626	78.636	11.689 12.769	1.00 25.16	7
	MOTA	411		PRO	52	26.510 27.553	79.138 80.091	13.270	1.00 24.54	6
	ATOM	412			52 52	26.917	77.763	12.974	1.00 25.24	6
60	MOTA	413			52	28.264	77.888	13.708	1.00 26.09	6
	ATOM	414 415			52	28.804	79.217	13.257	1.00 23.35	6
	MOTA MOTA	416		PRO	52	25.900	76.915	13.722	1.00 25.71	6
	ATOM	417		PRO	52	25.877	75.687	13.542	1.00 21.61	8 7
65	ATOM	418		SER	53	25.044	77.497	14.556	1.00 24.03	6
	MOTA	419			53	23.991	76.773 76.711	15.239 16.758	1.00 23.03	6
	MOTA	420			53 53	24.105 24.778	75.495	17.094	1.00 42.46	8
	MOTA	421		SER SER	53 53	22.681	77.460	14.854	1.00 24.85	6
70	MOTA	422 423		SER	53	22.681	78.673	14.691	1.00 23.68	8
70	MOTA MOTA	424		TYR	54	21.658	76.689	14.614	1.00 24.52	7
	AT ON		- ••							

	ATO:	4 426 CB TYP		20.333 77.167 14.212 1.00 26.29 6 20.050 76.886 12.729 1.00 26.92 6
	ATON		₹ 54	18.612 76.998 12.274 1.00 30.15 6
5	ATON ATON			17.719 77.905 12.825 1.00 29.18 6
	ATOM			16.407 78.006 12.409 1.00 31.26 6
	ATOM	431 CE2 TYR		18.104 76.166 11.280 1.00 31.67 6 16.796 76.217 10.855 1.00 31.66
	ATOM		54	15 050 77 151 14 150 31.00
10	ATOM ATOM			14.624 77.219 11.038 1.00 34.53 8
***	ATOM			19.378 76.450 15.167 1.00 24.84 6
	ATOM			19.300 75.210 15.129 1.00 22.53 B
	ATOM	437 CA ARG	55	17 864 76 650 17 070
15	ATOM		55	18.242 77.157 18.480 1.00 25.95 6
10	ATOM ATOM		55	17.478 76.340 19.551 1.00 23.98 6
	ATOM		55 55	17.651 76.982 20.918 1.00 35.38 6
	ATOM	442 CZ ARG	55	16.821 76.365 21.956 1.00 27.47 7 17.278 75.530 22.879 1.00 23.10
20	ATOM	443 NH1 ARG	55	19 570 75 700 00 00 00 00
20	MOTA	444 NH2 ARG	55	16.370 75.209 22.904 1.00 30.00 7 16.418 75.049 23.778 1.00 32.66 7
	MOTA MOTA	445 C ARG	55	16.434 77.103 16.802 1.00 27.49 6
	ATOM	446 O ARG 447 N PHE	55 56	16.275 78.312 16.569 1.00 22.62 8
	ATOM	448 CA PHE	56	15.455 76.174 16.781 1.00 23.78 7
25	MOTA	449 CB PHE	56	14.092 76.636 16.510 1.00 21.92 6 13.716 76.495 15.036 1.00 25.99 6
	MOTA	450 CG PHE	56	13 919 75 121 14 000 1.00 23.33 6
	ATOM	451 CD1 PHE	56	15.019 74.653 13.897 1.00 20.84 6
	ATOM ATOM	452 CD2 PHE 453 CE1 PHE	56	12.705 74.319 14.264 1.00 20.31 6
30	ATOM	453 CE1 PHE 454 CE2 PHE	56 56	15.103 73.415 13.283 1.00 21.52 6
	ATOM	455 CZ PHE	56 56	12.768 73.077 13.680 1.00 18.36 6 13.973 72.616 13.159 1.00 18.38
	MOTA	456 C PHE	56	12 005
	ATOM	457 O PHE	56	13 454 74 022 17 001
35	ATOM	458 N LYS	57	11.865 76.340 17.423 1.00 22.42 8
33	ATOM ATOM	459 CA LYS 460 CBA LYS	57	10.735 75.659 18.054 1.00 24.34 6
	ATOM	460 CBA LYS 461 CBB LYS	57 57	9.892 76.620 18.881 0.50 28.51 6
	ATOM	462 CGA LYS	57	9.822 76.727 18.669 0.50 22.87 6 10.656 77.298 20.010 0.50 33.64 6
40	MOTA	463 CGB LYS	57	9 760 76 200 10 600
40	ATOM	464 CDA LYS	57	11.436 76.342 20.892 0.50 40.75 6
	ATOM ATOM	465 CDB LYS 466 CEA LYS	57 53	8.631 77.186 20.798 0.50 26.90 6
	ATOM	467 CEB LYS	57 57	12.612 76.990 21.603 0.50 43.07 6
4.5	MOTA	468 NZA LYS	57	9.138 76.604 22.092 0.50 29.79 6 12.703 76.630 23.044 0.50 51.71 7
45	MOTA	469 NZB LYS	57	12.703 76.630 23.044 0.50 51.71 7 8.050 76.265 23.060 0.50 36.22 7
	ATOM ATOM	470 C LYS	57	9.950 74.923 16.969 1.00 21.30 6
	ATOM	471 O LYS 472 N ALA	57	9.436 75.551 16.052 1.00 19.46 8
	ATOM	472 N A <u>la</u> 473 CA Ala	58 58	9.928 73.588 16.945 1.00 18.23 7
50	ATOM	474 CB ALA	58	9.341 72.864 15.821 1.00 15.74 6 9.612 71.361 16.094 1.00 9.09 6
	ATOM	475 C ALA	58	7 841 77 074 15 074 1.00 9.09 6
	ATOM ATOM	476 O ALA	58	7.067 73.064 16.574 1.00 18.04 8
	ATOM	477 N ASN 478 CA ASN	59	7.392 73.126 14.367 1.00 18.31 7
55	ATOM	478 CA ASN 479 CB ASN	59 59	5.986 73.071 14.019 1.00 23.04 6
	ATOM	480 CG ASN	59	5.222 74.301 13.612 1.00 32.39 6 5.880 75.643 13.665 1.00 38.26 6
	ATOM	481 OD1 ASN	59	5 955 76 270 14 706
	ATOM	482 ND2 ASN	59	6.426 76.066 12.529 1.00 43.39 7
60	ATOM ATOM	483 C ASN	59	5.825 72.052 12.867 1.00 24.07 6
	ATOM	484 O ASN 485 N ASN	59 60	6.794 71.476 12.365 1.00 21.25 8
	ATOM	485 n asn 486 ca asn	60 60	4.582 71.833 12.484 1.00 24.40 7
	ATOM	487 CB ASN	60	4.192 70.823 11.519 1.00 31.47 6
<i>6</i> E	ATOM	488 CGA ASN	60	1.00 31.40 6
65	ATOM	489 CGB ASN	60	2.272 69.776 10.274 0.50 31.26 6 2.221 72.272 10.814 0.50 35.72 6
	ATOM ATOM	490 OD1 ASN	60	2.337 68.582 10.597 0.50 22.52 8
	ATOM	491 OD1 ASN 492 ND2 ASN	60 60	2.985 73.240 10.768 0.50 33.04 8
	ATOM	493 ND2 ASN	60 60	1.863 70.175 9.070 0.50 26.04 7
70	ATOM	494 C ASN	60	0.932 72.391 10.483 0.50 39.47 7 5.006 70.943 10.234 1.00 29.05 6
	ATOM	495 O ASN	60	
				5.645 69.986 9.780 1.00 32.27 8

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	497 CAA ASN 498 CAB ASN 499 CBA ASN 500 CBB ASN 501 CGA ASN 502 CGB ASN	61 61 61 61 61	5.098 72.153 5.863 72.487 5.857 72.367 5.564 73.955 5.403 73.671 4.101 74.127 5.608 74.882	8.529 0.50 28.68 8.477 0.50 29.13 8.150 0.50 26.19 7.806 0.50 30.25 7.792 0.50 27.01 8.678 0.50 32.36
10	ATOM ATOM ATOM ATOM ATOM	504 OD1 ASN 505 ND2 ASN 506 ND2 ASN 507 C ASN	61 61 61 61	3.502 75.125 6.383 74.820 3.526 73.172 4.927 75.991 7.371 72.336	8.184 0.50 28.58
15	MOTA MOTA MOTA MOTA	508 O ASN 509 N ASP 510 CA ASP 511 CB ASP 512 CG ASP	61 62 62 62 62	8.030 72.535 7.932 71.978 9.373 71.842 9.749 72.284 9.620 73.782	7.617 1.00 21.46 8 9.767 1.00 24.89 9.941 1.00 21.37 11.372 1.00 16.89 11.538 1.00 26.20
20	ATOM ATOM ATOM ATOM ATOM	513 OD1 ASP 514 OD2 ASP 515 C ASP 516 O ASP 517 N SER	62 62 62 62 63	9.824 74.549 9.276 74.273 9.887 70.439 11.104 70.209 9.011 69.477	10.570 1.00 20.81 8 12.611 1.00 17.90 8 9.645 1.00 18.69 6 9.654 1.00 20.50 8
25	ATOM ATOM ATOM ATOM ATOM	518 CA SER 519 CB SER 520 OG SER 521 C SER 522 O SER	63 63 63 63 63	9.434 68.132 8.268 67.164 7.506 67.018 10.196 68.204 10.015 69.160	9.015 1.00 19.84 6 8.811 1.00 22.04 6 10.009 1.00 20.02 8 7.682 1.00 23.89 6
30	ATOM ATOM ATOM ATOM ATOM	523 N GLY 524 CA GLY 525 C GLY 526 O GLY 527 N GLU	64 64 64 64 65	11.056 67.195 11.769 67.191 13.272 66.965 13.744 66.564	6.911 1.00 17.92 8 7.467 1.00 19.50 7 6.190 1.00 22.23 6 6.340 1.00 19.81 6 7.399 1.00 18.93 8
35	ATOM ATOM ATOM ATOM ATOM	528 CA GLU 529 CBA GLU 530 CBB GLU 531 CGA GLU	65 65 65 65	13.980 67.226 15.428 67.013 15.934 66.562 15.933 66.446 16.507 65.158	5.238 1.00 17.01 7 5.269 1.00 21.39 6 3.901 0.50 13.64 6 3.947 0.50 23.81 6 3.813 0.50 15.71 6
40	MOTA MOTA MOTA	532 CGB GLU 533 CDA GLU 534 CDB GLU 535 OE1 GLU 536 OE1 GLU	65 65 65 65 65	15.409 65.059 16.656 64.679 15.898 63.965 17.428 65.263 16.578 64.271	3.602 0.50 32.15 6 2.381 0.50 22.33 6 4.520 0.50 40.56 6 1.586 0.50 22.70 8 5.525 0.50 41.83 8
45	ATOM ATOM ATOM ATOM ATOM	537 OE2 GLU 538 OE2 GLU 539 C GLU 540 O GLU 541 N TYR	65 65 65 65 66	15.991 63.686 15.624 62.758 16.155 68.324 15.756 69.325 17.172 68.268	2.014 0.50 31.04 8 4.278 0.50 46.02 8 5.593 1.00 21.56 6 5.007 1.00 21.41 8
50	ATOM ATOM ATOM ATOM ATOM	542 CA TYR 543 CB TYR 544 CG TYR 545 CD1 TYR 546 CE1 TYR	66 66 66 66	17.966 69.483 17.954 69.984 16.620 70.563 15.605 69.686 14.369 70.147	6.691 1.00 17.91 6 8.129 1.00 17.39 6 8.534 1.00 18.08 6 8.957 1.00 18.56 6
55	ATOM ATOM ATOM ATOM ATOM	547 CD2 TYR 548 CE2 TYR 549 CZ TYR 550 OH TYR 551 C TYR	66 66 66 66	16.348 71.921 15.102 72.382 14.124 71.516 12.872 71.939 19.379 69.231	9.323 1.00 16.48 6 8.485 1.00 18.23 6 8.867 1.00 18.37 6 9.279 1.00 18.98 6 9.624 1.00 14.14 8 6.212 1.00 13.96 6
60	ATOM ATOM ATOM ATOM ATOM ATOM	552 O TYR 553 N THR 554 CA THR 555 CB THR 556 OG1 THR	66 67 67 67	19.923 68.135 20.010 70.228 21.374 70.138 21.514 69.844 20.669 70.737	6.353 1.00 18.14 8 5.568 1.00 17.95 7 5.117 1.00 18.06 6 3.599 1.00 22.52 6 2.835 1.00 16.85 8
65	ATOM ATOM ATOM ATOM	557 CG2 THR 558 C THR 559 O THR 560 N CYS 561 CA CYS	67 67 67 68 68	21.215 68.371 22.044 71.508 21.354 72.515 23.354 71.540 24.099 72.792	3.309 1.00 17.46 6 5.384 1.00 18.76 6 5.567 1.00 17.47 8 5.389 1.00 19.74 7 5.597 1.00 23.50 6
70	ATOM ATOM ATOM ATOM ATOM	562 C CYS 563 O CYS 564 CB CYS 565 SG CYS 566 N GLN	68 68 68 69	25.382 72.759 25.791 71.712 24.434 73.082 25.675 71.985 25.975 73.920	4.758 1.00 23.12 6 4.279 1.00 25.07 8 7.055 1.00 18.70 6 7.798 1.00 23.45 16 4.534 1.00 24.47 7

	ATOM	567	CA	GLN	69	27.174	74.121	3.770	1.00 24.99	6
	MOTA	568	CB	GLN	69	26.909	74.344	2.264	1.00 27.22	6
	MOTA	569		GLN	69	28.155	74.057	1.419	1.00 25.14	6
E	MOTA	570		GLN	69	27.857	74.022	-0.065	1.00 32.43	6
5	MOTA	571	OE:	GLN	69	26.710	74.166	-0.487	1.00 31.34	8
	MOTA MOTA	572 573	C NE	GLN GLN	69 69	28.896 27.901	73.814 75.383	-0.874 4.266	1.00 27.89 1.00 27.60	7 6
	ATOM	574		GLN	69	27.289	76.352	4.734	1.00 27.80	8
	ATOM	575	N	THR	70	29.206	75.318	4.115	1.00 28.73	7
10	ATOM	576	CA	THR	70	30.059	76.465	4.439	1.00 32.10	6
	MOTA	577	СВ	THR	70	31.125	76.153	5.491	1.00 33.36	6
	MOTA	578	OG I	THR	70	30.619	75.311	6.553	1.00 45.26	8
	MOTA	579	CG2	THR	70	31.453	77.444	6.210	1.00 50.20	6
	MOTA	580	С	THR	70	30.737	76.890	3.138	1.00 32.77	6
15	ATOM	581	0	THR	70	30.680	76.170	2.130	1.00 30.75	8
	ATOM	582	N	GLY	71	31.472	78.007	3.175	1.00 31.83	7
	ATOM	583	CA	GLY	71 71	32.224	78.469	2.033	1.00 27.97	6
	ATOM ATOM	584 585	C O	GLY GLY	71	33.376 33.938	77.544 77.668	1.690 0.596	1.00 29.94 1.00 32.37	6 8
20	ATOM	586	N	GLN	72	33.842	76.707	2.594	1.00 24.86	7
20	ATOM	587	CA	GLN	72	34.920	75.779	2.457	1.00 27.14	6
	ATOM	588	CB	GLN	72	35.868	75.974	3.667	1.00 27.31	6
	MOTA	589	CG	GLN	72	36.291	77.451	3.825	1.00 30.51	6
	ATOM	590	CD	GLN	72	36.961	77.995	2.567	1.00 30.53	6
25	MOTA	591	OE1	GLN	72	37.981	77.441	2.161	1.00 39.95	8
	ATOM	592		GLN	72	36.402	79.014	1.944	1.00 31.16	7
	ATOM	593	С	GLN	72	34.530	74.305	2.441	1.00 29.60	6
	ATOM	594	0	GLN	72	35.419	73.442	2.578	1.00 30.82	8
30	MOTA	595 596	N	THR	73 73	33.248	73.954	2.380	1.00 25.83	7 6
30	MOTA MOTA	597	CA CB	THR	73 73	32.861 32.278	72.549 72.135	2.426 3.792	1.00 26.62 1.00 26.64	6
	ATOM	598		THR	73	31.226	73.051	4.138	1.00 27.54	8
	ATOM	599	CG2		73	33.313	72.124	4.897	1.00 28.16	6
	ATOM	600	C	THR	73	31.824	72.223	1.371	1.00 26.31	6
35	ATOM	601	0	THR	73	31.210	73.110	0.776	1.00 28.00	8
	ATOM	602	N	SER	74	31.685	70.927	1.074	1.00 28.62	7
	ATOM	603	CA	SER	74	30.592	70.605	0.112	1.00 29.44	6
	MOTA	604	CB	SER	74	31.020	69.470	-0.803	1.00 30.45	6
40	MOTA	605	OG	SER	74	31.407	68.399	0.034	1.00 41.05	8
40	ATOM ATOM	606 607	C O	SER SER	74 74	29.366 29.461	70.395 70.438	0.992 2.228	1.00 26.65 1.00 25.57	6 8
	ATOM	608	N	LEU	75	28.178	70.281	0.442	1.00 29.47	7
	ATOM	609	CA	LEU	75	26.915	70.163	1.158	1.00 25.10	6
	ATOM	610	CB	LEU	75	25.749	70.141	0.159	1.00 27.83	6
45	ATOM	611	CG	LEU	75	24.348	70.136	0.777	1.00 27.24	6
	MOTA	612	CD1	LEU	75	23.888	71.554	1.094	1.00 24.13	6
	ATOM	613	CD2	LEU	75	23.349	69.420	-0.133	1.00 24.42	6
	ATOM	614	С	LEU	75	26.884	68.973	2.087	1.00 25.84	6
	ATOM	615	0	LEU	75	27.300	67.858	1.711	1.00 22.45	8
50	ATOM	616	N	SER	76	26.376	69.158	3.315	1.00 23.31	7
	MOTA	617	CA.	SER	76 76	26.357	68.009	4.219	1.00 25.20	6
	MOTA	618	CB OG	SER	76 76	25.916	68.402	5.644	1.00 26.64	6 8
	ATOM ATOM	619 620	C	SER SER	76	24.514 25.346	68.663 66.955	5.624 3.738	1.00 29.43 1.00 23.00	6
55	MOTA	621	Ö	SER	76	24.431	67.304	3.006	1.00 21.02	8
00	MOTA	622	N	ASP	77	25.506	65.739	4.241	1.00 22.24	7
	MOTA	623	CA	ASP	77	24.493	64.712	4.094	1.00 26.03	6
	ATOM	624	CB	ASP	77	24.907	63.362	4.683	1.00 20.27	6
	MOTA	625	CG	ASP	77	25.914	62.676	3.758	1.00 25.73	6
60	ATOM	626	OD1	ASP	77	25.821	62.893	2.541	1.00 23.79	8
	MOTA	627		ASP	77	26.769	61.954	4.292	1.00 28.92	8
	MOTA	628	С	ASP	77	23.267	65.191	4.929	1.00 25.85	6
	ATOM	629	0	ASP	77	23.423	65.904	5.914	1.00 24.00	8
6 E	MOTA	630	N	PRO	78 70	22.098	64.758	4.492	1.00 27.37	7
65	ATOM	631	CD	PRO	78 79	21.917 20.849	63.917	3.275	1.00 26.84	6
	MOTA ATOM	632 633	CA CB	PRO PRO	78 78	19.795	65.130 64.592	5.098 4.141	1.00 25.42 1.00 28.38	6 6
	ATOM	634	CG	PRO	78	20.453	63.586	3.272	1.00 27.24	6
	ATOM	635	C	PRO	78	20.575	64.556	6.479	1.00 25.28	6
70	ATOM	636	ō	PRO	78	21.006	63.459	6.820	1.00 23.68	8
	ATOM	637	N	VAL	79	19.833	65.331	7.265	1.00 20.24	7

	ATOM	638	CA.	VAL	79	19.287	64.861	8.535	1.00 18.86	6
	ATOM	639		VAL	79	19.850	_	9.783	1.00 19.49	6
	MOTA	640	CG1	VAL	79	19.042	65.239	11.046	1.00 22.25	6
_	ATOM	641	CG2	VAL	79	21.275	64.959	10.036	1.00 21.95	6
5	MOTA	642		VAL	79	17.777		8.399	1.00 19.76	6
	MOTA	643		VAL	79	17.283		8.076	1.00 22.34	8
	MOTA	644		HIS	80	17.024	63.955	8.566	1.00 19.43	7
	ATOM	645		HIS	80	15.584	63.976	8.387	1.00 18.11	6
10	ATOM	646		HIS	80	15.130	62.621	7.784	1.00 26.87	6
10	MOTA	647		HIS	80	13.712	62.754	7.293	1.00 31.93	6
	atom atom	648 649		HIS	80 80	13.194	62.983	6.069	1.00 27.05 1.00 34.35	6
	ATOM	650		HIS	80	12.637 11.525	62.697 62.847	8.176 7.480	1.00 34.35	7 6
	ATOM	651		HIS	80	11.831	63.016	6.210	1.00 34.80	7
15	ATOM	652		HIS	80	14.865	64.187	9.718	1.00 23.08	6
	ATOM	653		HIS	80	15.096	63.496	10.709	1.00 23.37	8
	ATOM	654		LEU	81	13.953	65.138	9.747	1.00 19.18	7
	ATOM	655	CA	LEU	81	13.244	65.478	10.957	1.00 21.58	6
•	MOTA	656	CB	LEU	81	13.567	66.937	11.331	1.00 18.20	6
20	MOTA	657	CG	LEU	81	12.847	67.381	12.605	1.00 18.21	6
	ATOM	658		LEU	81	13.496	66.708	13.812	1.00 19.39	6
	MOTA	659		LEU	81	12.865	68.912	12.696	1.00 14.76	6
	MOTA	660	C	LEU	81	11.747	65.255	10.783	1.00 19.36	6
25	ATOM	661	0	LEU	81	11.225	65.543	9.720	1.00 20.96	8
25	ATOM	662	N	THR	82	11.100	64.689	11.793	1.00 19.61	7
	MOTA MOTA	663 664	CA CB	THR	82 82	9.642 9.316	64.463 62.950	11.680	1.00 18.45	6
	ATOM	665		THR	82	9.907	62.351	11.683	1.00 25.98	6
	ATOM	666		THR	82	7.795	62.775	10.527 11.666	1.00 18.89 1.00 24.98	8 6
30	ATOM	667	c	THR	82	8.971	65.100	12.891	1.00 24.98	6
	ATOM	668	ŏ	THR	82	9.248	64.735	14.035	1.00 14.79	8
	ATOM	669	N	VAL	83	8.075	66.045	12.647	1.00 16.23	7
	ATOM	670	CA	VAL	83	7.451	66.758	13.753	1.00 16.97	6
	ATOM	671	CB	VAL	83	7.559	68.282	13.530	1.00 12.81	6
35	MOTA	672	CG1	VAL	83	7.051	68.972	14.799	1.00 15.92	6
	MOTA	673		VAL	83	8.986	68.760	13.246	1.00 11.78	6
	ATOM	674	С	VAL	83	6.020	66.264	13.892	1.00 19.97	6
	ATOM	675	0	VAL	83	5.261	66.329	12.918	1.00 18.57	8
40	ATOM	676	N	LEU	84	5.686	65.756	15.075	1.00 16.89	7
40	ATOM	677 678	CA	LEU	84	4.372	65.188	15.312	1.00 19.89	6
	MOTA MOTA	679	CB CG	LEU	84 84	4.621 5.491	63.786	15.890	1.00 18.15	6
	ATOM	680		LEU	84	5.927	62.863 61.690	15.021 15.868	1.00 23.40 1.00 25.20	6 6
	ATOM	681		LEU	84	4.752	62.396	13.758	1.00 20.46	6
45	ATOM	682	c	LEU	84	3.487	66.016	16.228	1.00 22.29	6
	ATOM	683	0	LEU	84	3.928	66.891	16.975	1.00 23.90	8
	ATOM	684	N	PHE	85	2.189	65.750	16.218	1.00 21.03	7
	ATOM	685	CA	PHE	85	1.254	66.444	17.111	1.00 22.92	6
	MOTA	686	CB	PHE	85	0.399	67.431	16.333	1.00 21.76	6
50	ATOM	687	CG	PHE	85	-0.440	68.350	17.184	1.00 27.90	6
	MOTA	688	CD1		85	0.103	69.013	18.266	1.00 28.30	6
	ATOM	689	CD2		85	-1.787	68.533	16.899	1.00 26.61	6
	ATOM	690	CE1		85	-0.664	69.874	19.040	1.00 29.65	6
55	ATOM	691	CE2		85	-2.559	69.386	17.668	1.00 25.61	6
J J	ATOM	692	CZ	PHE	85	-1.996	70.047	18.733	1.00 28.75	6
	MOTA	693	C	PHE	85	0.455	65.399	17.852	1.00 21.99	6
	ATOM ATOM	694 695	N O	PHE GLU	85 86	-0.642 1.023	65.000 64.883	17.426	1.00 22.11	8
	ATOM	696	CA	GLU	86	0.421	63.762	18.938 19.702	1.00 20.76	7
60	ATOM	697	CB	GLU	86	1.142	62.463	19.702	1.00 18.04 1.00 20.84	6 6
•	ATOM	698	CG	GLU	86	0.711	61.815	17.911	1.00 25.05	6
	ATOM	699	CD	GLU	86	1.647	61.048	17.019	1.00 23.05	6
	ATOM	700	OE1		86	2.719	60.507	17.416	1.00 46.14	8
	ATOM	701		GLU	86	1.429	60.893	15.765	1.00 40.77	8
65	ATOM	702		GLU	86	0.694	64.026	21.176	1.00 18.46	6
	ATOM	703		GLU	86	1.588	64.839	21.462	1.00 16.67	8
	ATOM	704		TRP	87	0.031	63.408	22.156	1.00 12.60	7
	MOTA	705		TRP	87	0.328	63.631	23.553	1.00 13.01	6
7 0	MOTA	706		TRP	87	-0.808	63.056	24.411	1.00 18.40	6
70	MOTA	707		TRP	87	-1.922	64.023	24.687	1.00 21.87	6
	MOTA	708	CD2	TRP	87	-1.812	65.176	25.521	1.00 21.14	6

	ATOM ATOM ATOM	710 CE3 TRP	87	-3.065 65.805 25.526 1.00 24.31 6 -0.767 65.738 26.255 1.00 24.84 6
5	ATOM	712 NEI TRP	87	-3.216 63.985 24.231 1.00 22.52 6 -3.907 65.069 24.734 1.00 22.53 7
J	MOTA MOTA		87 87	-3.303 66.966 26.266 1.00 29.91 6
	ATOM	715 CH2 TRP	87	-0.998 66.890 26.987 1.00 29.83 6 -2.254 67.499 26.970 1.00 29.09 6
	MOTA MOTA	716 C TRP 717 O TRP	87	1.599 62.967 24.068 1.00 15.44 6
10	ATOM	717 O TRP 718 N LEU	87 88	2.178 63.499 25.018 1.00 16.68 8 2.036 61.873 23.447 1.00 14.44 7
	ATOM ATOM	719 CA LEU	88	3.153 61.051 23.861 1.00 20.07 6
	ATOM	720 CB LEU 721 CG LEU	88 88	2.596 59.942 24.783 1.00 17.49 6
15	ATOM	722 CD1 LEU	88	3.608 59.303 25.769 1.00 16.97 6 4.062 60.299 26.830 1.00 17.38 6
10	MOTA MOTA	723 CD2 LEU 724 C LEU	88 88	2.987 58.053 26.370 1.00 13.93 6
	MOTA	725 O LEU	88	3.889 60.399 22.677 1.00 20.44 6 3.255 59.857 21.752 1.00 19.65 8
	ATOM ATOM	726 N VAL 727 CA VAL	89	5.218 60.517 22.620 1.00 18.11 7
20	MOTA	728 CBA VAL	89 89	5.998 59.926 21.542 1.00 14.66 6 6.686 61.029 20.699 0.50 7.52 6
	ATOM ATOM	729 CBB VAL	89	6.677 60.941 20.604 0.50 13.86 6
	ATOM	730 CG1 VAL 731 CG1 VAL	89 89	7.573 61.890 21.597 0.50 7.13 6
25	ATOM	732 CG2 VAL	89	5.696 61.409 19.543 0.50 15.87 6 7.501 60.486 19.531 0.50 3.91 6
23	ATOM ATOM	733 CG2 VAL 734 C VAL	89 89	7.264 62.090 21.402 0.50 18.65 6
	MOTA	735 O VAL	89	7.109 59.032 22.107 1.00 15.71 6 7.689 59.262 23.179 1.00 14.52 8
	ATOM ATOM	736 N LEU 737 CA LEU	90	7.379 57.958 21.386 1.00 15.13 7
30	ATOM	738 CB LEU	90 90	8.520 57.133 21.703 1.00 13.72 6 8.287 55.625 21.488 1.00 17.87 6
	ATOM	739 CG LEU	90	9.650 54.978 21.873 1.00 26.07 6
	MOTA ATOM	740 CD1 LEU 741 CD2 LEU	90 90	9.479 54.066 23.036 1.00 30.57 6
35	ATOM	742 C LEU	90	10.373 54.463 20.662 1.00 25.07 6 9.657 57.674 20.803 1.00 17.58 6
33	ATOM ATOM	743 O LEU 744 N GLN	90	9.611 57.517 19.576 1.00 14.46 8
	ATOM	745 CA GLN	91 91	10.673 58.298 21.412 1.00 15.83 7 11.745 58.908 20.623 1.00 17.70 6
	ATOM ATOM	746 CB GLN	91	12.252 60.238 21.264 1.00 15.03 6
40	ATOM	747 CG GLN 748 CD GLN	91 91	11.105 61.231 21.472 1.00 12.81 6
	ATOM	749 OE1 GLN	91	11.564 62.636 21.868 1.00 15.79 6 12.023 62.823 22.988 1.00 14.61 8
	ATOM ATOM	750 NE2 GLN 751 C GLN	91 91	11.409 63.610 20.984 1.00 16.27 7
A E	ATOM	752 O GLN	91	12.971 58.042 20.375 1.00 17.71 6 13.370 57.296 21.268 1.00 19.37 8
45	ATOM ATOM	753 N THR 754 CA THR	92	13.607 58.207 19.218 1.00 14.05 7
	ATOM	755 CB THR	92 92	14.853 57.488 18.934 1.00 19.01 6 14.562 56.225 18.089 1.00 16.40 6
	ATOM ATOM	756 OG1 THR	92	15.769 55.485 17.905 1.00 18.39 8
50	ATOM	757 CG2 THR 758 C THR	92 92	13.943 56.499 16.720 1.00 10.45 6
	ATOM ATOM	759 O THR	92	15.803 58.416 18.173 1.00 18.96 6 15.339 59.272 17.409 1.00 21.88 8
	ATOM	760 N PRO 761 CD PRO	93 93	17.095 58.153 18.251 1.00 18.78 7
55	ATOM	762 CA PRO	93	17.747 57.169 19.135 1.00 22.16 6 18.090 58.929 17.530 1.00 24.37 6
33	ATOM ATOM	763 CB PRO 764 CG PRO	93	19.352 58.803 18.371 1.00 24.99 6
	ATOM	764 CG PRO 765 C PRO	93 93	19.162 57.609 19.235 1.00 26.05 6 18.285 58.362 16.138 1.00 27.02 6
	ATOM ATOM	766 O PRO	93	18.852 59.019 15.248 1.00 27.04 8
60	ATOM	767 N HIS 768 CA HIS	94 94	17.978 57.069 15.960 1.00 24.22 7
	ATOM	769 CB HIS	94	18.114 56.421 14.651 1.00 25.72 6 19.444 55.690 14.439 1.00 20.09 6
	ATOM ATOM	770 CG HIS 771 CD2 HIS	94 94	20.639 56.587 14.595 1.00 21.67 6
e e	ATOM	772 ND1 HIS	94	21.161 57.530 13.798 1.00 23.30 6 21.380 56.595 15.754 1.00 27.49 7
65	ATOM ATOM	773 CE1 HIS	94	22.338 57.501 15.657 1.00 26.54 6
	ATOM	774 NE2 HIS 775 C HIS	94 94	22.211 58.078 14.482 1.00 32.10 7
	ATOM	776 O HIS	94	17.038 55.350 14.453 1.00 24.49 6 16.481 54.838 15.429 1.00 24.01 8
70	ATOM ATOM	777 N LEU 778 CA LEU	95 95	16.847 54.929 13.214 1.00 21.96 7
	ATOM	779 CB LEU	95	15.900 53.847 12.960 1.00 26.06 6 15.014 54.118 11.741 1.00 26.66 6
				1.00 20.00

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	782 CD: 783 C 784 O 785 N 786 CA	LEU 1 LEU 2 LEU LEU LEU GLU GLU	95 95 95 95 96 96	13.99 13.44 12.89 16.62 15.99 17.88 18.68	9 55.60 5 54.90 6 52.52 9 51.46 4 52.60 8 51.41	1 10.525 8 12.900 5 12.720 4 12.790 1 12.326	1.00 25.66 1.00 24.13 1.00 26.30 1.00 26.83 1.00 25.44	6 6 6 8
10	ATOM ATOM ATOM ATOM ATOM ATOM	787 CB 788 CG 789 CD 790 OE1 791 OE2 792 C	GTU GTU GTU GTU GTU	96 96 96 96 96 96	19.06 17.97 18.41 19.56 17.59	7 51.334 4 51.109 50.709 2 51.343	9.605 8.168 7.882 7.256	1.00 34.46 1.00 42.07 1.00 41.53 1.00 45.31	6 6 8 8
15	ATOM ATOM ATOM ATOM ATOM	793 O 794 N 795 CA 796 CB 797 CG	GLU PHE PHE PHE PHE	96 97 97 97 97	19.99! 20.52! 20.396 21.622 21.388 20.640	52.686 50.487 50.447 50.351	13.015 13.538 14.315 15.832	1.00 32.22 1.00 31.68 1.00 29.38 1.00 31.45 1.00 29.88	6 7 6 6
20	ATOM ATOM ATOM ATOM ATOM	798 CD1 799 CD2 800 CE1	PHE PHE PHE PHE PHE	97 97 97 97 97	19.256 21.311 18.557 20.622 19.244	51.580 52.503 52.624 53.545	16.386 17.131 16.971 17.719	1.00 28.91 1.00 19.88 1.00 27.06 1.00 23.29 1.00 23.27	6 6 6 6
25	MOTA MOTA MOTA MOTA MOTA	803 C 804 O 805 N 806 CA 807 CB	PHE PHE GLN GLN GLN	97 97 98 98 98	22.455 22.007 23.726 24.636 26.042	49.233 48.334 49.213 48.131	13.861 13.164 14.219 13.939	1.00 25.87 1.00 31.11 1.00 32.31 1.00 34.14 1.00 33.31	6 8 7 6
30	ATOM ATOM ATOM ATOM ATOM	808 CG 809 CD 810 OE1	GLN GLN GLN GLN GLN	98 98 98 98 98	26.207 25.763 26.455 24.603	49.422 48.712 47.828 49.088	13.635 12.356 11.097 10.589 10.563	1.00 38.15 1.00 45.65 1.00 49.99 1.00 52.58 1.00 53.06	6 6 8 7
35	ATOM ATOM ATOM ATOM ATOM	813 O 814 N 815 CA 816 CB	GLU GLU GLU	98 99 99 99	24.662 24.459 24.990 25.112 25.598	47.218 47.664 45.955 44.978 43.653	15.172 16.300 14.920 16.009 15.420	1.00 31.48 1.00 27.98 1.00 30.75 1.00 32.56 1.00 36.89	6 8 7 6 6
40	ATOM ATOM ATOM ATOM ATOM	818 CD 819 OE1 820 OE2 821 C	GLU GLU	99 99 99 99	25.204 24.771 23.802 25.400 26.130	42.392 41.288 40.573 41.148 45.551	16.141 15.184 15.521 14.118 16.980	1.00 44.86 1.00 48.45 1.00 53.90 1.00 50.56 1.00 31.14	6 8 8 6
45	ATOM ATOM ATOM ATOM ATOM	823 N 824 CA 825 C 826 O	GLY GLY GLY	99 100 100 100 100	27.136 25.919 26.874 26.643 27.082	46.048 45.571 46.123 47.541 47.931	16.475 18.275 19.217 19.696 20.789	1.00 31.94 1.00 32.19 1.00 31.10 1.00 31.51 1.00 30.30	8 7 6 6 8
50	ATOM ATOM ATOM ATOM	828 CA 829 CB 830 CG 831 CD	GTA GTA GTA GTA	101 101 101 101 101	25.948 25.675 24.949 25.777 24.984	48.369 49.746 50.452 50.676 51.520	18.921 19.297 18.148 16.889 15.895	1.00 34.41 1.00 34.07 1.00 37.86 1.00 48.38 1.00 49.17	7 6 6 6
55	ATOM ATOM ATOM ATOM ATOM ATOM	835 O 6		101 101 101 101 102 102	24.251 25.046 24.783 24.086 24.747 23.870	52.408 51.333 49.848 48.888 51.057 51.303	16.385 14.669 20.537 20.886 21.107	1.00 58.51 1.00 48.56 1.00 33.06 1.00 27.70 1.00 31.92	8 8 6 8 7
60	ATOM ATOM ATOM ATOM ATOM	838 CB 7 839 OG1 7 840 CG2 7 841 C 7	THR THR THR THR	102 102 102 102 102	24.508 25.546 23.532 22.582 22.650	52.161 51.438 52.577 51.944 52.932	23.341 24.021 24.441 21.721	1.00 32.85 1.00 35.75 1.00 36.79 1.00 35.82 1.00 32.54	6 8 6 6
65	ATOM ATOM ATOM ATOM ATOM	843 N I 844 CA I	LE LE LE	103 103 103 103 103	21.431 20.162 19.131 17.776 19.669	51.329 51.939 50.873 51.496	22.014 21.590 21.163 20.828	1.00 30.03 1.00 28.53 1.00 25.40 1.00 26.58 1.00 25.47	8 7 6 6
70	ATOM ATOM ATOM	848 CD1 I 849 C I	LE LE	103 103 103	18.739 19.624	49.003 52.753	19.438 1 22.767 1	1.00 21.79 1.00 19.73 1.00 25.27 1.00 23.06	6 6 6 8

82

6

MOTA 851 N MET 104 19.443 54.059 22.591 1.00 24.90 MOTA 852 MET 18.893 CA 104 54.913 23.639 1.00 21.55 MOTA 853 СВ MET 104 19.797 56.097 23.963 1.00 33.48 ATOM 854 CG MET 104 20.810 55.826 25.101 1.00 29.68 5 MOTA 855 SD MET 104 21.940 57.256 25.242 1.00 46.02 16 MOTA 856 22.667 1.00 31.10 CE MET 104 57.216 23.589 6 MOTA 857 С MET 104 17.528 55.456 23.215 1.00 21.27 ATOM 858 MET 0 104 17.374 55.991 22.106 1.00 22.96 8 ATOM 105 859 N LEU 16.503 55.242 24.027 1.00 20.55 7 10 ATOM 860 CA LEU 105 15.134 55.668 23.728 1.00 22.33 6 ATOM 861 CB LEU 105 14.192 54.450 23.550 1.00 14.66 6 ATOM 862 CG T.EII 105 14.713 53.389 22.561 1.00 18.89 6 MOTA 863 CD1 LEU 105 13.796 52.178 22.489 1.00 19.44 6 ATOM 864 CD2 LEU 105 14.882 54.056 21,186 1.00 18.70 6 15 ATOM 865 С LEU 105 14.567 56.559 1.00 20.15 24.817 MOTA 866 0 15.050 LEU 105 56.506 25.950 1.00 18.39 ATOM 867 N ARG 106 13.523 57.324 24.483 1.00 18.25 7 ATOM 868 CA ARG 106 12.912 58.174 25.516 1.00 17.87 6 ATOM 869 CB ARG 59.553 106 13.607 25.508 1.00 14.96 6 20 ATOM 870 CG ARG 106 12.834 60.597 26.290 1.00 16.79 13.699 ATOM 871 CD ARG 106 61.788 26.757 1.00 19.51 6 MOTA 872 NE ARG 106 13.334 62.927 26.025 1.00 23.46 ATOM 873 CZ ARG 106 12.990 64.174 26.065 1.00 24.43 6 ATOM 874 NH1 ARG 106 12.923 64.892 27.176 1.00 25.93 25 ATOM 106 875 NH2 ARG 12.697 64.795 24.936 1.00 18.72 7 ATOM 876 C ARG 106 11.422 58.321 25.304 1.00 18.56 6 ATOM 877 10.998 0 ARG 106 58.479 24.142 1.00 20.43 8 ATOM 878 N CYS 107 10.642 58.246 26.378 1.00 15.23 ATOM 879 CA CYS 107 9.189 58.419 1.00 14.89 26.292 6 30 ATOM 880 C CYS 107 8.934 59.891 26.583 1.00 15.28 6 ATOM 881 9.296 0 CYS 107 60.294 27.690 1.00 15.96 ATOM 882 CB CYS 107 8.438 57.565 27.322 1.00 14.55 6 ATOM 883 SG 107 CYS 6.691 57.368 27.013 1.00 13.91 16 ATOM 884 N HIS 108 8.446 60.653 25.604 1.00 15.07 7 35 MOTA 885 CA 108 HIS 8.334 62.103 25.811 1.00 11.91 6 ATOM 886 CB HIS 108 9.190 62.757 24.708 1.00 16.03 ATOM 887 CG HIS 108 9.119 64.240 24.572 1.00 16.94 6 CD2 HIS ATOM 888 108 9.068 65.023 23.462 1.00 17.64 6 65.108 66.350 ATOM 889 ND1 HIS 108 9.103 1.00 17.41 25.657 7 40 ATOM 890 CE1 HIS 108 9.034 25.215 1.00 17.37 6 ATOM 891 NE2 HIS 108 9.021 66.333 23.895 1.00 20.00 7 ATOM 892 С HIS 108 6.925 62.647 25.733 1.00 11.83 6 ATOM 893 0 HIS 108 6.224 62.361 24.762 1.00 12.54 8 ATOM 894 N SER 109 63.502 6.515 26.654 1.00 13.70 7 45 MOTA 895 CA 109 SER 5.160 64.091 26.605 1.00 11.70 6 ATOM 896 CB SER 109 4.583 64.134 28.041 1.00 13.47 6 ATOM 897 OG SER 109 5.609 1.00 16.16 64.845 28.800 8 ATOM 898 С SER 109 5.190 65.459 25.970 1.00 14.21 6 ATOM 899 0 SER 109 6.180 66.232 25.903 1.00 14.63 8 50 ATOM 900 N TRP 110 4.047 65.804 25.381 1.00 16.58 7 24.708 ATOM 901 CA TRP 110 3.860 67.102 1.00 16.04 6 ATOM 902 2.480 CB TRP 110 67.158 24.072 1.00 18.73 ATOM 903 CG TRP 110 2.187 68.425 23.306 1.00 21.24 6 MOTA CD2 TRP 904 110 1.135 69.339 23.589 1.00 20.70 6 55 ATOM 905 CE2 TRP 110 1.193 70.361 22.616 1.00 25.92 ATOM 906 CE3 TRP 110 0.112 69.372 24.549 1.00 24.16 6 ATOM 907 CD1 TRP 110 2.827 68.908 22.214 1.00 22.22 6 MOTA 908 NE1 TRP 110 2.233 70.069 21.765 1.00 22.81 7 0.276 MOTA 909 CZ2 TRP 110 71.404 22.568 1.00 24.18 6 60 MOTA 910 CZ3 TRP -0.781 110 70.434 24.509 1.00 30.15 6 ATOM 911 CH2 TRP 110 -0.698 71.433 23.526 1.00 31.04 6 ATOM 912 С TRP 110 4.082 68.245 25.681 1.00 14.44 6 ATOM 913 0 TRP 110 3.665 68.219 26.852 1.00 17.08 ATOM 914 LYS N 111 4.928 69.199 25.294 1.00 19.42 7 65 ATOM 915 CA LYS 111 5.347 70.325 26.115 1.00 19.40 6 MOTA 916 CB LYS 111 4.131 71.241 26.418 1.00 21.00 MOTA 917 CG LYS 111 3.583 71.904 25.155 1.00 24.94 б ATOM CD 918 LYS 111 2.124 72.287 25.337 1.00 34.17 6 ATOM 919 CE LYS 111 1.952 73.719 25.781 1.00 37.49 6 70 MOTA 920 NZ LYS 111 2.783 74.668 24.987 1.00 52.66 7 MOTA 921 C LYS 5.940 111 69.921 27.450 1.00 20.33

	MOTA MOTA MOTA MOTA	922 O 923 N 924 CA 925 CB	LYS ASP ASP ASP	111 112 112 112	5.905 6.444 6.989 8.242	68.695 68.233	27.602 28.861	1.00 18.28 1.00 20.31	8 7 6
5	MOTA ATOM ATOM ATOM	926 CG 927 OD:	ASP 1 ASP 2 ASP ASP	112 112 112 112 112	9.306 9.700 9.719 6.015	68.737 67.545 69.588	28.155 28.119 27.360	1.00 31.39 1.00 39.68 1.00 35.00	6 8 8 6
10	MOTA MOTA ATOM	930 O 931 N 932 CA 933 CB	ASP LYS LYS	112 113 113 113	6.426 4.731 3.792 2.352	68.475 67.889 67.721 67.432	31.148 29.785	1.00 23.42 1.00 23.10 1.00 22.35	8 7 6 6
15	MOTA MOTA MOTA MOTA MOTA MOTA	934 CG 935 CD 936 CE 937 NZ 938 C	LYS LYS LYS LYS	113 113 113 113 113	1.758 0.232 -0.269 -0.196	68.574 69.780 71.075	29.659 29.608 28.816 29.554	1.00 28.34 1.00 32.92 1.00 33.55	6 6 7
20	ATOM ATOM ATOM ATOM	939 O 940 N 941 CD 942 CA	LYS PRO PRO PRO	113 114 114 114	4.352 4.890 4.288 3.701 4.923	65.603 66.761 67.928	31.748 31.264 33.066 33.768 33.957	1.00 19.86 1.00 21.45 1.00 20.08 1.00 16.95 1.00 17.00	6 8 7 6 6
25	ATOM MOTA ATOM ATOM	943 CB 944 CG 945 C 946 O	PRO PRO PRO	114 114 114 114	4.548 4.169 4.451 3.237	66.292 67.733 64.405 64.125	35.342 35.176 33.636 33.512	1.00 19.22 1.00 21.34 1.00 16.83 1.00 16.01	6 6 8
30	ATOM ATOM ATOM ATOM ATOM ATOM	947 N 948 CA 949 CB 950 CG 951 CD1	LEU LEU LEU LEU	115 115 115 115 115	5.414 5.081 5.769 5.790	63.483 62.104 61.879 60.498	33.560 33.215 31.856 31.231	1.00 15.95 1.00 17.10 1.00 16.83 1.00 21.64	7 6 6
	MOTA MOTA MOTA MOTA		LEU LEU LEU VAL	115 115 115 115 116	4.399 6.777 5.606 6.788 4.839	60.132 60.486 61.116 61.200 60.105	30.733 30.043 34.226 34.569 34.630	1.00 19.24 1.00 19.80 1.00 21.13 1.00 18.84 1.00 20.51	6 6 8 7
35	ATOM ATOM ATOM ATOM	956 CA 957 CB 958 CG1	VAL VAL VAL	116 116 116 116	5.314 4.787 5.313 3.257	59.073 59.277 60.547 59.328	35.545 36.971 37.644 36.998	1.00 20.40 1.00 18.72 1.00 22.67 1.00 22.12	6 6 6
40	ATOM MOTA ATOM MOTA	960 C 961 O 962 N 963 CA	VAL VAL LYS LYS	116 116 117 117	4.807 3.910 5.268 4.760	57.703 57.682 56.615 55.290	35.073 34.223 35.693 35.381	1.00 19.73 1.00 20.76 1.00 17.34 1.00 20.33	6 8 7 6
4 5	ATOM ATOM ATOM ATOM ATOM	964 CB 965 CG 966 CD 967 CE	LYS LYS LYS	117 117 117 117	3.271 3.115 1.793 0.798	55.182 54.927 55.445 54.314	35.802 37.301 37.832 38.056	1.00 21.74 1.00 24.43 1.00 32.69 1.00 40.27	6 6 6
50	ATOM ATOM ATOM ATOM	968 NZ 969 C 970 O 971 N 972 CA	LYS LYS LYS VAL VAL	117 117 117 118 118	-0.568 4.956 4.026 6.181 6.542	54.865 54.936 54.535 55.063 54.798	38.266 33.914 33.234 33.417 32.039	1.00 44.06 1.00 18.58 1.00 24.35 1.00 20.45 1.00 19.15	7 6 8 7 6
55	ATOM ATOM ATOM ATOM ATOM	977 0	VAL VAL VAL	118 118 118 118 118	7.756 8.199 7.408 6.868 7.606	55.643 55.396 57.129 53.330 52.717		1.00 12.17 1.00 18.94 1.00 16.75 1.00 18.58 1.00 17.16	6 6 6 6 8
60	ATOM ATOM ATOM ATOM ATOM	979 CA		119 119 119 119 119	6.307 6.527 5.291 4.770 5.695	52.803 51.425 50.523 50.410 49.123	30.711 30.335 30.367 31.693 29.872	1.00 15.94 1.00 16.50 1.00 19.59 1.00 23.11 1.00 24.83	7 6 6 8 6
65	ATOM ATOM ATOM ATOM ATOM	983 C 984 O 985 N 986 CA	THR THR PHE PHE PHE	119 119 120 120 120	7.053 6.436 8.121 8.616 10.122	51.424 52.130 50.679 50.608 50.797	28.881 28.095 28.643 27.259 27.240	1.00 17.81 1.00 14.36 1.00 14.86 1.00 13.85 1.00 15.51	6 8 7 6
70	ATOM ATOM ATOM ATOM ATOM		PHE PHE PHE PHE	120 120 120 120 120	10.553 10.748 10.792 11.186 11.230	52.230 52.701 53.051 54.002 54.367	27.463 28.750 26.381 28.953 26.578	1.00 13.38 1.00 20.15 1.00 20.08 1.00 17.14 1.00 22.12	6 6 6 6

5	MOTA MOTA MOTA MOTA MOTA MOTA	99 99 99 99 99	4 C 5 O 6 N 7 C 8 C 9 C	PHE PHE PHE PHE PHE	120 120 121 121 121 121		11.42 8.27 8.64 7.62 7.27 5.79	9 49.21 0 48.22 6 49.16 7 47.86 9 47.82	6 26.72 1 27.40 6 25.57 8 25.01 1 24.61	1 1.00 17.13 7 1.00 14.78 5 1.00 16.20 1 1.00 18.83 6 1.00 13.50	8 6 8 7 6 6
10	MOTA MOTA MOTA MOTA MOTA MOTA		1 CE 2 CE 3 CE 4 CZ		121 121 121 121		4.368 4.208 3.409 3.260 2.843	46.963 49.524 47.173 48.445	9 26.01° 1 26.334 27.006 3 27.313 5 27.660	7 1.00 17.37 4 1.00 18.44 5 1.00 19.78 3 1.00 22.69 0 1.00 15.74	6 6 6 6
15	MOTA MOTA MOTA MOTA MOTA	100 100 100 100 100 101	6 O 7 N 8 CA 9 CB	GLN	121 121 122 122 122		8.074 8.351 8.333 8.959 10.396	48.454 46.253 45.880 45.379	22.987 3 23.480 22.203 22.317	7 1.00 15.63 1.00 19.35 1.00 19.90 7 1.00 16.32	8 7 6 6
20	MOTA MOTA MOTA MOTA MOTA	1012 1012 1013 1014 1015	CD COE NE C		122 122 122 122 122 122		10.784 12.050 12.423 12.700 8.067	43.764 43.461 43.396 44.774	21.247 22.374 20.153 21.609	1.00 21.98 1.00 19.18 1.00 24.51 1.00 15.34	6 8 7 6
25	ATOM ATOM ATOM ATOM ATOM	1016 1017 1018 1019	N CA CB CG	ASN ASN ASN ASN ASN	123 123 123 123 123 123		7.789 7.474 6.542 7.241 8.228	44.931 43.975 42.708 43.130	20.439 19.859 19.332 18.244	1.00 18.98 1.00 22.95 1.00 19.57 1.00 26.31	8 7 6 6 6
30	ATOM ATOM ATOM ATOM ATOM	1021 1022 1023 1024 1025	ND2	ASN ASN ASN GLY GLY	123 123 123 123 124 124		8.013 9.375 5.397 4.911 4.951	44.053 42.463 43.643 42.525 44.632	18.213 20.803 20.918 21.579	1.00 19.76 1.00 28.57 1.00 21.02 1.00 19.19 1.00 19.77	8 7 6 8 7
35	ATOM ATOM ATOM ATOM ATOM	1026 1027 1028 1029 1030	С 0 N	GLY GLY LYS LYS	124 124 125 125		3.852 4.159 3.210 5.405 5.830	44.516 43.885 43.658 43.610 42.997	22.495 23.844 24.611 24.133 25.379	1.00 16.41 1.00 14.85 1.00 15.05 1.00 13.81 1.00 21.18	6 8 7 6
40	ATOM ATOM ATOM ATOM ATOM	1031 1032 1033 1034	CG CD CE NZ	LYS LYS LYS	125 125 125 125 125		6.700 6.934 7.406 7.925 8.822	41.738 41.032 39.587 38.989 37.818	25.247 26.559 26.281 27.587 27.330	1.00 14.85 1.00 16.28 1.00 22.51 1.00 30.62 1.00 36.72	6 6 6 7
4 5	ATOM ATOM ATOM ATOM	1035 1036 1037 1038 1039	C N CA CB	LYS LYS SER SER SER	125 125 126 126 126		6.725 7.648 6.385 7.107 6.355	44.014 44.525 44.216 45.241 45.459	26.121 25.509 27.393 28.155 29.485	1.00 18.20 1.00 19.98 1.00 17.62 1.00 20.03 1.00 23.22	6 8 7 6 6
50	ATOM ATOM ATOM ATOM ATOM	1040 1041 1042 1043 1044	OG C O N CA	SER SER SER GLN GLN	126 126 126 127 127		7.317 8.541 8.842 9.490 10.898	45.773 44.823 43.657 45.718 45.515	30.466 28.389 28.647 28.254 28.408	1.00 38.12 1.00 17.85 1.00 21.31 1.00 17.16 1.00 17.45	8 6 8 7 6
55	ATOM ATOM ATOM ATOM ATOM ATOM	1045 1046 1047 1048 1049 1050	CB CG CD OE1 NE2 C		127 127 127 127 127 127		11.723 11.352 11.497 12.606 10.436 11.386	46.073 45.419 43.912 43.416 43.130 46.251	27.225 25.897 25.927 26.116 25.773 29.661	1.00 20.82 1.00 18.56 1.00 24.44 1.00 31.62 1.00 19.15	6 6 6 8 7
60	ATOM ATOM ATOM ATOM ATOM	1051 1052 1053 1054 1055	O N CA CB	GLN LYS LYS LYS LYS	127 128 128 128 128		12.439 10.643 11.070 12.177 12.683	45.929 47.285 48.048 49.034 49.882	30.179 30.032 31.216 30.842 32.013	1.00 20.94 1.00 18.25 1.00 21.18 1.00 23.10 1.00 21.83	6 8 7 6 6
65	ATOM ATOM ATOM ATOM ATOM	1056 1057 1058 1059 1060	CD CE NZ C	LYS LYS LYS LYS LYS	128 128 128 128 128	:	13.739 14.048 15.081 9.884 9.193	50.905 51.746 52.794 48.844	31.589 32.870 32.574 31.754	1.00 24.67 1.00 18.23 1.00 27.02 1.00 24.24 1.00 24.93	6 6 7 6
70	ATOM ATOM ATOM	1061 1062 1063	N CA	PHE PHE PHE	129 129 129 129		9.678 8.708	49.481 48.822 49.695 48.926	33.062 33.695	1.00 20.79 1.00 21.39 1.00 24.45 1.00 25.50	8 7 6 6

	ATOM	1064	CG PHI	E 129	6.772	49.837	35.327	1.00 25.51	6
	ATOM	1065			5.799		34.762	1.00 19.40	6
	MOTA	1066			7.002	49.928	36.700	1.00 29.98	6
_	ATOM	1067			5.026		35.535	1.00 25.00	6
5	MOTA	1068	CE2 PHI		6.249		37.491	1.00 28.84	6
	ATOM	1069			5.262	51.574	36.902	1.00 32.29	6
	MOTA MOTA	1070 1071	C PHI		9.480 10.388	50.577	34.687 35.359	1.00 27.88	6
	ATOM	1071	N SEI		9.134	50.049 51.846	34.853	1.00 30.99 1.00 26.67	8 7
10	ATOM	1073	CA SEI		9.779	52.641	35.917	1.00 24.98	6
	ATOM	1074	CB SEI		11.025	53.344	35.422	1.00 21.29	6
	ATOM	1075	OG SEI		11.271	54.465	36.250	1.00 25.72	8
	ATOM	1076	C SEI		8.777	53.667	36.434	1.00 24.39	6
	ATOM	1077	O SER	130	8.123	54.285	35.576	1.00 24.91	8
15	ATOM	1078	N HIS		8.668	53.889	37.730	1.00 22.12	7
	MOTA	1079	CA HIS		7.710	54.901	38.204	1.00 23.65	6
	ATOM	1080	CB HIS		7.604	54.918	39.737	1.00 28.35	6
	ATOM	1081	CG HIS		6.859	53.706	40.197	1.00 23.57	6
20	ATOM	1082	CD2 HIS		7.307	52.509	40.642	1.00 18.55	6
20	MOTA ATOM	1083 1084	ND1 HIS		5.478	53.666	40.170	1.00 26.69	7
	ATOM	1085	NE2 HIS		5.095 6.173	52.478 51.764	40.617	1.00 16.65	6
	ATOM	1086	C HIS		8.108	56.314	37.814	1.00 23.94 1.00 23.89	7 6
	ATOM	1087	O HIS		7.261	57.205	37.712	1.00 26.21	8
25	ATOM	1088	N LEU		9.426	56.548	37.689	1.00 20.21	7
	ATOM	1089	CA LEU		9.886	57.900	37.480	1.00 20.70	6
	ATOM	1090	CB LEU		10.630	58.361	38.760	1.00 30.28	6
	ATOM	1091	CG LEU		10.022	58.084	40.148	1.00 26.56	6
	ATOM	1092	CD1 LEU	132	11.073	58.316	41.229	1.00 29.07	6
30	ATOM	1093	CD2 LEU	132	8.814	58.980	40.435	1.00 24.99	6
	MOTA	1094	C LEU		10.762	58.144	36.279	1.00 22.94	6
	ATOM	1095	O LEU		10.794	59.326	35.900	1.00 22.01	8
	ATOM	1096	N ASP		11.541	57.181	35.778	1.00 21.75	7
35	ATOM	1097	CA ASP		12.469	57.401	34.679	1.00 24.62	6
33	ATOM	1098	CB ASP		13.560	56.327	34.854	1.00 29.71	6
	ATOM ATOM	1099 1100	CG ASP OD1 ASP		14.734	56.321	33.915	1.00 32.90	6
	ATOM	1101	ODI ASP		14.837 15.597	57.254 55.394	33.083	1.00 32.91 1.00 36.01	8
	ATOM	1102	C ASP		11.843	57.230	34.000 33.296	1.00 25.88	8 6
40	ATOM	1103	O ASP		11.419	56.136	32.940	1.00 24.36	8
	ATOM	1104	N PRO		11.857	58.261	32.460	1.00 24.65	7
	ATOM	1105	CD PRO		12.347	59.620	32.778	1.00 22.97	6
	ATOM	1106	CA PRO	134	11.293	58.185	31.112	1.00 24.00	6
4 ==	ATOM	1107	CB PRO		10.889	59.662	30.870	1.00 24.02	6
45	ATOM	1108	CG PRO		11.987	60.433	31.544	1.00 23.04	6
	MOTA	1109	C PRO		12.256	57.764	30.017	1.00 22.11	6
	ATOM	1110	O PRO	134	11.970	57.930	28.824	1.00 19.00	8
	ATOM	1111	N THR	135	13.420	57.212	30.350	1.00 21.43	7
50	ATOM	1112	CA THR	135	14.424	56.805	29.401	1.00 24.98	6
30	ATOM ATOM	1113 1114	CB THR	135	15.748	57.584	29.593	1.00 27.24	6
	ATOM	1115	OG1 THR	135 135	16.331	57.065	30.796	1.00 24.99 1.00 26.07	8
	ATOM	1116	C THR	135	15.461 14.747	59.069 55.312	29.706 29.451	1.00 28.07	6 6
	ATOM	1117	O THR	135	14.445	54.629	30.423	1.00 25.38	8
55	ATOM	1118	N PHE	136	15.267	54.790	28.347	1.00 20.63	7
	ATOM	1119	CA PHE	136	15.549	53.391	28.150	1.00 20.00	6
	MOTA	1120	CB PHE	136	14.343	52.706	27.523	1.00 25.47	6
	ATOM	1121	CG PHE	136	14.408	51.250	27.170	1.00 25.61	6
	MOTA	1122	CD1 PHE	136	14.528	50.270	28.121	1.00 27.00	6
60	MOTA	1123	CD2 PHE	136	14.332	50.847	25.841	1.00 27.45	6
	MOTA	1124	CE1 PHE	136	14.571	48.929	27.787	1.00 32.62	6
	ATOM	1125	CE2 PHE	136	14.385	49.516	25.490	1.00 28.46	6
	MOTA	1126	CZ PHE	136	14.493	48.549	26.463	1.00 30.41	6
C E	ATOM	1127	C PHE	136	16.796	53.197	27.297	1.00 24.00	6
65	ATOM	1128	O PHE	136	16.952	53.801	26.230	1.00 24.50	8
	MOTA	1129	N SER	137	17.665	52.294	27.730	1.00 21.97	7
	ATOM	1130	CA SER	137	18.914	52.010	27.050	1.00 26.52	6
	ATOM	1131	CB SER	137	20.120	52.418	27.908	1.00 30.03	6
70	ATOM ATOM	1132 1133	OG SER	137 137	20.769 19.128	53.559 50.507	27.412	1.00 44.19	8 6
, 0	ATOM	1134	O SER	137	18.911	49.694	26.840 27.721	1.00 27.38 1.00 27.33	8
		+	- DAK	13,	20.711	42.037	~ 1 · 1 4 ±	1.00 21.33	J

5	ATON ATON ATON ATON ATON ATON ATON	1136 1137 1138 1139 1140 1141	N ILL CA ILL CB ILL CG2 ILL CG1 ILL CD1 ILL C ILL O ILL	E 138 E 138 E 138 E 138 E 138 E 138	19.60 20.00 19.10 19.60 17.67 16.81 21.47	04 48.80 99 48.17 99 46.74 99 48.19 17 48.15 17 48.87	6 25.343 6 24.193 8 23.941 7 24.472 5 23.223 5 24.926	1.00 29.4 1.00 33.3 1.00 27.2 1.00 30.5 1.00 29.5 1.00 29.8	6 6 8 6 3 6 5 6
10	ATOM ATOM ATOM ATOM	1143 1144 1145 1146	N PRO CD PRO CA PRO CB PRO	139 139 139 139	21.76 22.34 22.01 23.77 24.38	5 48.476 8 47.938 6 48.398	25.837 27.184 25.598	1.00 31.73 1.00 32.73 1.00 33.85	1 7 3 6 5 6
15	ATOM ATOM ATOM ATOM ATOM	1148 1149 1150	CG PRO C PRO O PRO N GLN CA GLN	139 139 140	23.24 24.03 23.32 24.97 25.28	8 48.384 0 47.160 4 46.160 4 47.208	27.950 24.741 24.888 23.827	1.00 34.99 1.00 35.63 1.00 38.22 1.00 36.97	6 6 8 7
20	ATOM ATOM ATOM ATOM ATOM	1153 1154 1155	CB GLN CG GLN CD GLN OE1 GLN NE2 GLN	140 140 140 140	26.22 27.51 27.88 28.14	3 45.124 8 45.802 3 45.282 5 44.084	23.631 24.088 25.468 25.593	1.00 35.17 1.00 43.87 1.00 49.77 1.00 56.21 1.00 57.44	6 6
25	ATOM ATOM ATOM ATOM	1157 1158 1159 1160	C GLN O GLN N ALA CA ALA	140 140 140 141 141	27.883 24.066 23.67 23.473 22.28	45.418 7 44.284 8 46.111	26.468 22.362 22.693 21.391 20.694	1.00 57.25 1.00 34.61 1.00 33.34 1.00 29.80 1.00 30.02	7 6 8 7 6
30	ATOM ATOM ATOM ATOM ATOM	1162 1163 1164	CB ALA C ALA O ALA N ASN CA ASN	141 141 141 142 142	21.778 22.561 23.650 21.528 21.642	46.745 44.400 44.270 43.582	19.774 19.832 19.263 19.665 18.738	1.00 27.89 1.00 29.52 1.00 29.60 1.00 30.60	6 6 8 7
35	ATOM MOTA ATOM ATOM ATOM	1167 (1168 (1169)	CB ASN CG ASN DD1 ASN ND2 ASN C ASN	142 142 142 142 142	21.985 21.012 19.838 21.479	41.139 40.749 40.423 40.739	19.453 20.534 20.268 21.781	1.00 31.55 1.00 30.39 1.00 31.63 1.00 27.57 1.00 33.23	6 6 8 7
40	ATOM ATOM ATOM ATOM	1171 0 1172 1 1173 0 1174 0	ASN HIS HIS HIS HIS	142 143 143 143	20.357 19.453 20.223 19.075 19.262	43.168	17.936 18.122 17.134 16.266 15.272	1.00 32.33 1.00 29.09 1.00 29.40 1.00 28.82 1.00 24.51	6 8 7 6 6
45	MOTA MOTA MOTA MOTA MOTA	1176 C 1177 N 1178 C	CG HIS CD2 HIS CD1 HIS CE1 HIS CE2 HIS	143 143 143 143 143	20.360 20.704 21.278 22.117 21.794	40.234 41.420 39.328 39.927 41.202	14.295 13.740 13.822 13.008	1.00 31.72 1.00 33.88 1.00 32.86 1.00 31.84	6 6 7 6
50	MOTA MOTA MOTA MOTA	1180 C 1181 O 1182 N 1183 C	HIS HIS SER A SER	143 143 144 144	17.747 16.696 17.812 16.557	41.202 40.857 41.098 40.412 40.128	16.976 16.366 18.221	1.00 31.48 1.00 26.62 1.00 25.96 1.00 20.85 1.00 24.82	7 6 8 7 6
	MOTA MOTA MOTA MOTA MOTA	1184 C 1185 O 1186 C 1187 O 1188 N	G SER	144 144 144 144 145	16.839 17.739 15.976 14.775	38.979 39.389 41.423 41.518	19.915 20.930 19.474 19.755	1.00 30.28 1.00 39.11 1.00 24.89 1.00 25.22	6 8 6 8
55	ATOM ATOM ATOM ATOM	1189 CZ 1190 CZ 1191 CC 1192 CZ	A HIS B HIS F HIS D2 HIS	145 145 145 145	16.746 16.306 17.474 18.145 17.620	44.762 44.212	19.811 : 20.302 : 21.534 :	1.00 20.33 1.00 19.38 1.00 19.40 1.00 18.37 1.00 18.22	7 6 6 6
60	ATOM ATOM ATOM ATOM ATOM	1194 CE 1195 NE 1196 C	O1 HIS E1 HIS E2 HIS HIS	145 145 145 145	19.493 19.768 18.643 15.589	43.965 43.492 43.412 44.553	21.627 1 22.829 1 23.525 1	1.00 16.22 1.00 23.55 1.00 26.33 1.00 21.05 1.00 22.05	6 7 6 7 6
65	ATOM ATOM ATOM ATOM	1197 O 1198 N 1199 CA 1200 CB 1201 OG	SER	145 146 146 146 146	15.013 15.569 14.833 15.075 16.442	43.997 44.649 44.009	18.848 1 17.440 1 16.363 1 14.986 1	.00 21.86 .00 20.66 .00 19.96 .00 20.48	8 7 6 6
70	ATOM ATOM ATOM	1202 C 1203 O 1204 N 1205 CA	SER SER GLY GLY	146 146 147 147	13.339 12.915 12.556 11.123	44.596 1 43.614 1 45.578 1	l6.656 1 l7.287 1 l6.197 1	.00 25.61 .00 20.51 .00 22.06 .00 16.70 .00 20.49	8 6 8 7 6

	ATOM	1206	С	GLY	147	10.385	46.714	16.555	1.00 22.63	6
	ATOM	1207	ō	GLY	147	10.982	47.762	16.332	1.00 16.09	8
	ATOM	1208	N	ASP	148	9.111	46.560	16.951	1.00 20.62	7
	MOTA	1209	CA	ASP	148	8.324	47.777	17.121	1.00 21.57	6
5	MOTA	1210	CB	ASP	148	6.882	47.579	16.674	1.00 28.99	6
	MOTA	1211	CG	ASP	148	6.819	47.144	15.219	1.00 41.07	6
	ATOM	1212		ASP	148	7.849	47.338	14.540	1.00 39.21	8 8
	MOTA	1213		ASP	148	5.763 8.315	46.620 48.214	14.808 18.590	1.00 39.40 1.00 20.72	6
10	ATOM	1214 1215	С 0	ASP ASP	148 148	7.817	47.469	19.447	1.00 20.72	8
10	ATOM ATOM	1216	N	TYR	149	8.822	49.440	18.798	1.00 16.97	7
	ATOM	1217	CA	TYR	149	8.811	49.966	20.164	1.00 18.60	6
	ATOM	1218	CB	TYR	149	10.193	50.587	20.472	1.00 16.94	6
	ATOM	1219	CG	TYR	149	11.272	49.534	20.606	1.00 18.45	6
15	ATOM	1220	CD1	TYR	149	11.901	48.928	19.528	1.00 19.27	6
	ATOM	1221	CE1		149	12.877	47.948	19.737	1.00 20.18	6
	ATOM	1222	CD2		149	11.672	49.162	21.879	1.00 18.36 1.00 15.60	6 6
	ATOM	1223	CE2		149 149	12.636 13.238	48.216 47.606	22.116 21.027	1.00 13.60	6
20	ATOM ATOM	1224 1225	CZ OH	TYR TYR	149	14.211	46.660	21.253	1.00 18.41	8
20	ATOM	1226	C	TYR	149	7.767	51.061	20.355	1.00 15.78	6
	MOTA	1227	ō	TYR	149	7.539	51.859	19.450	1.00 15.86	8
	ATOM	1228	N	HIS	150	7.196	51.126	21.559	1.00 15.01	7
	ATOM	1229	CA	HIS	150	6.247	52.171	21.925	1.00 12.99	6
25	ATOM	1230	CB	HIS	150	4.849	51.980	21.372	1.00 11.96	6
	MOTA	1231	CG	HIS	150	3.942	51.032	22.117	1.00 17.71	6
	ATOM	1232		HIS	150	2.944 3.988	51.295	23.004	1.00 16.09 1.00 11.60	6 7
	MOTA	1233 1234		HIS HIS	150 150	3.988	49.660 49.103	21.971 22.716	1.00 16.95	6
30	MOTA MOTA	1235		HIS	150	2.407	50.057	23.370	1.00 19.22	ž
30	ATOM	1236	C	HIS	150	6.263	52.270	23.462	1.00 13.37	6
	ATOM	1237	ō	HIS	150	6.922	51.448	24.129	1.00 12.78	8
	ATOM	1238	N	CYS	151	5.680	53.355	23.957	1.00 14.21	7
	ATOM	1239	CA	CYS	151	5.670	53.559	25.414	1.00 15.38	6
35	ATOM	1240	С	CYS	151	4.301	53.982	25.880	1.00 16.27	6
	MOTA	1241	0	CYS	151	3.422	54.404	25.132	1.00 15.15 1.00 16.85	8 6
	MOTA	1242	CB	CYS	151 151	6.746 6.581	54.562 56.269	25.856 25.248	1.00 14.82	16
	MOTA MOTA	1243 1244	SG N	CYS	152	4.080	53.805	27.186	1.00 17.41	7
40	ATOM	1245	CA	THR	152	2.875	54.223	27.862	1.00 17.27	6
10	ATOM	1246	СВ	THR	152	1.899	53.131	28.305	1.00 21.80	6
	MOTA	1247	OG1	THR	152	2.527	52.212	29.205	1.00 17.53	8
	MOTA	1248	CG2		152	1.356	52.388	27.075	1.00 17.12	6
4.5	MOTA	1249	C	THR	152	3.346	54.989	29.127	1.00 19.83	6
45	MOTA	1250	0	THR	152	4.471	54.724	29.600	1.00 16.21	8 7
	MOTA	1251	N CA	GLY GLY	153 153	2.496 2.815	55.913 56.706	29.534 30.731	1.00 17.84 1.00 20.33	6
	ATOM ATOM	1252 1253	C	GLY	153	1.647	57.605	31.108	1.00 18.60	6
	ATOM	1254	ō	GLY	153	0.779	57.915	30.293	1.00 19.87	8
50	ATOM	1255	N	ASN	154	1.603	58.000	32.373	1.00 20.99	7
	MOTA	1256	CA	ASN	154	0.560	58.815	32.959	1.00 20.36	6
	MOTA	1257	CB	asn	154	0.512	58.556	34.478	1.00 26.77	6
	MOTA	1258	CG	ASN	154	-0.800	57.928	34.897	1.00 40.91	6
r r	MOTA	1259		ASN	154	-1.700	58.580	35.441	1.00 46.67	8
55	ATOM	1260		ASN	154	-0.927 0.879	56.639 60.300	34.633 32.817	1.00 40.24 1.00 22.51	7 6
	ATOM ATOM	1261 1262	С 0	ASN ASN	154 154	1.973	60.685	33.272	1.00 22.31	8
	ATOM	1263	N	ILE	155	-0.018	61.067	32.202	1.00 19.40	7
	ATOM	1264	CA	ILE	155	0.198	62.514	32.139	1.00 22.27	6
60	ATOM	1265	CB	ILE	155	0.210	63.116	30.731	1.00 26.29	6
	MOTA	1266	CG2	ILE	155	0.327	64.640	30.831	1.00 23.31	6
	ATOM	1267		ILE	155	1.367	62.544	29.899	1.00 28.16	6
	MOTA	1268		ILE	155	1.371	62.874	28.434	1.00 29.42	6
<i>C</i> E	MOTA	1269	C	ILE	155	-0.974	63.089	32.941	1.00 27.67	6
65	ATOM	1270	O N	ILE	155 156	-2.112 -0.732	62.726 63.838	32.639 34.020	1.00 24.10 1.00 33.10	8 7
	MOTA MOTA	1271 1272	N CA	GLY GLY	156	-1.942	64.285	34.780	1.00 33.10	6
	ATOM	1273	C	GLY	156	-2.447	63.053	35.527	1.00 38.80	6
	ATOM	1274	ō	GLY	156	-1.659	62.512	36.299	1.00 43.91	8
70	ATOM	1275	N	TYR	157	-3.655	62.573	35.307	1.00 41.47	7
	ATOM	1276	CA	TYR	157	-4.182	61.357	35.894	1.00 43.65	6

	ATOM	1277	СВ	TYR	157	-5.381	61.642	36.832	1.00 51.51	6
	ATOM	1278	CG	TYR	157	-5.020	62.592	37.961	1.00 57.42	6
	ATOM	1279	CD1	TYR	157	-5.523	63.885	37.982	1.00 60.45	6
	ATOM	1280		TYR	157	-5.179	64.765	38.992	1.00 62.57	6
5	ATOM	1281		TYR	157	-4.140	62.204	38.963	1.00 61.00	6
_	ATOM	1282	CE2	TYR	157	-3.788	63.079	39.982	1.00 63.03	6
	ATOM	1283	CZ	TYR	157	-4.313	64.353	39.986	1.00 63.56	6
	ATOM	1284	OH	TYR	157	-3.979	65.237	40.984	1.00 66.68	8
	ATOM	1285	C	TYR	157	-4.676	60.351	34.849	1.00 41.96	6
10	ATOM	1286	ō	TYR	157	-5.445	59.420	35.115	1.00 41.33	8
10	ATOM	1287	N	THR	158	-4.298	60.547	33.594	1.00 36.77	7
	ATOM	1288	CA	THR	158	-4.722	59.693	32.496	1.00 30.71	6
	ATOM	1289	СВ	THR	158	-5.260	60.597	31.364	1.00 30.82	6
	ATOM	1290	OG1		158	-6.237	61.471	31.942	1.00 30.47	8
15	ATOM	1291	CG2	THR	158	-5.851	59.819	30.207	1.00 29.21	6
	ATOM	1292	c	THR	158	-3.532	58.944	31.912	1.00 25.66	6
	ATOM	1293	ō	THR	158	-2.521	59.609	31.642	1.00 24.50	8
	ATOM	1294	N	LEU	159	-3.689	57.664	31.609	1.00 21.00	7
	ATOM	1295	CA	LEU	159	-2.617	56.924	30.960	1.00 21.01	6
20	ATOM	1296	СВ	LEU	159	-2.737	55.435	31.284	1.00 26.53	6
20	ATOM	1297	CG	LEU	159	-1.601	54.487	30.958	1.00 27.15	6
	ATOM	1298		LEU	159	-0.323	54.817	31.713	1.00 25.15	6
	ATOM	1299		LEU	159	-1.979	53.036	31.316	1.00 28.75	6
	ATOM	1300	c	LEU	159	-2.654	57.179	29.461	1.00 22.04	6
25	ATOM	1301	ŏ	LEU	159	-3.711	57.248	28.844	1.00 22.64	8
20	ATOM	1302	N	PHE	160	-1.484	57.396	28.855	1.00 20.79	7
	ATOM	1303	CA	PHE	160	-1.430	57.576	27.409	1.00 19.10	6
	ATOM	1304	CB	PHE	160	-0.821	58.946	27.060	1.00 20.91	6
	ATOM	1305	CG	PHE	160	-1.848	60.034	27.216	1.00 19.50	6
30	ATOM	1306		PHE	160	-1.971	60.676	28.442	1.00 24.86	6
•	ATOM	1307		PHE	160	-2.645	60.409	26.156	1.00 21.03	6
	ATOM	1308		PHE	160	-2.903	61.709	28.588	1.00 29.44	6
	ATOM	1309		PHE	160	-3.582	61.421	26.296	1.00 19.89	6
	ATOM	1310	CZ	PHE	160	-3.704	62.074	27.529	1.00 25.34	6
35	ATOM	1311	C	PHE	160	-0.521	56.513	26.794	1.00 17.36	6
	ATOM	1312	0	PHE	160	0.346	55.982	27.504	1.00 18.36	8
	ATOM	1313	N	SER	161	-0.753	56.240	25.521	1.00 17.60	7
	ATOM	1314	CA	SER	161	0.087	55.302	24.785	1.00 14.63	6
	MOTA	1315	CB	SER	161	-0.744	54.150	24.188	1.00 20.14	6
40	MOTA	1316	OG	SER	161	0.115	53.054	23.901	1.00 21.55	8
	ATOM	1317	С	SER	161	0.662	56.037	23.561	1.00 18.96	6
	MOTA	1318	0	SER	161	-0.101	56.753	22.894	1.00 19.79	8
	ATOM	1319	N	SER	162	1.921	55.796	23.232	1.00 16.19	7
	ATOM	1320	CA	SER	162	2.518	56.404	22.049	1.00 16.74	6
45	ATOM	1321	CB	SER	162	4.029	56.678	22.233	1.00 16.78	6
	ATOM	1322	OG	SER	162	4.801	55.530	21.900	1.00 21.00	8
	ATOM	1323	С	SER	162	2.322	55.485	20.845	1.00 18.24	6
	ATOM	1324	0	SER	162	1.949	54.305	20.987	1.00 16.85	8
	ATOM	1325	N	LYS	163	2.535	56.027	19.652	1.00 17.96	7
50	ATOM	1326	CA	LYS	163	2.484	55.203	18.445	1.00 17.36	6
	ATOM	1327	CB	LYS	163	2.369	55.957	17.133	1.00 20.94	6
	MOTA	1328	CG	LYS	163	1.228	56.885	16.902	1.00 25.34	6
	MOTA	1329	CD	LYS	163	-0.128	56.271	16.685	1.00 29.02	6
	ATOM	1330	CE	LYS	163	-0.954	57.131	15.721	1.00 42.35	6
55	MOTA	1331	NZ	LYS	163	-0.495	58.558	15.692	1.00 38.14	7
	MOTA	1332	С	LYS	163	3.821	54.466	18.391	1.00 17.27	6
	MOTA	1333	0	LYS	163	4.817	54.906	18.978	1.00 16.54	8
	ATOM	1334	N	PRO	164	3.840	53.348	17.696	1.00 18.39	7
	ATOM	1335	CD	PRO	164	2.702	52.743	16.952	1.00 20.79	6
60	ATOM	1336	CA	PRO	164	5.060	52.572	17.546	1.00 19.84	6
	ATOM	1337	CB	PRO	164	4.545	51.177	17.142	1.00 17.33	6
	ATOM	1338	CG	PRO	164	3.254	51.416	16.475	1.00 21.76	6
	ATOM	1339	С	PRO	164	6.032	53.169	16.528	1.00 19.62	6
	ATOM	1340	0	PRO	164	5.723	53.942	15.619	1.00 19.46	8
65	ATOM	1341	N	VAL	165	7.295	52.833	16.674	1.00 17.22	7
	ATOM	1342	CA	VAL	165	8.427	53.162	15.841	1.00 20.36	6
	ATOM	1343	CB	VAL	165	9.405	54.190	16.450	1.00 20.84	6
	MOTA	1344	CG1	VAL	165	10.418	54.643	15.404	1.00 20.46	6
	MOTA	1345	CG2	VAL	165	8.699	55.475	16.899	1.00 23.72	6
70	ATOM	1346	С	VAL	165	9.173	51.833	15.590	1.00 22.05	6
	MOTA	1347	0	VAL	165	9.532	51.094	16.499	1.00 22.10	8

	ATOM	1348	3 N	THR	166	9.444	51.549	14.320	1.00 24.93	
	MOTA	1349				10.111				
	MOTA	1350				9.631				
	ATOM	1351								
5				1 THR		9.737				
5	ATOM	1352				8.180			1.00 23.71	(
	ATOM	1353	3 C	THR	166	11.611	50.597	13.909	1.00 25.06	•
	MOTA	1354	0	THR	166	11.985	51.536			,
	MOTA	1355	N	ILE		12.362				
	ATOM	135€			167	13.784				
10	ATOM	1357			167					٠
10						14.088				6
	ATOM	1358		2 ILE	167	15.588			1.00 26.68	6
	MOTA	1359		1 ILE	167	13.415	51.472	16.825	1.00 26.56	6
	ATOM	1360) CD	1 ILE	167	13.946	52.318	17.939	1.00 30.83	6
	MOTA	1361	. с	ILE	167	14.416				ě
15	ATOM	1362		ILE	167	14.013				
	ATOM	1363		THR	168	15.412				8
										7
	MOTA	1364			168	16.083			1.00 27.27	6
	ATOM	1365			168	15.945	47.266	11.622	1.00 31.88	6
	MOTA	1366	OG	1 THR	168	14.565	47.371	11.277	1.00 32.11	8
20	ATOM	1367	CG	2 THR	168	16.462	45.894		1.00 34.54	6
	ATOM	1368	С	THR	168	17.575		13.501	1.00 28.53	
	ATOM	1369		THR	168	18.190				6
	ATOM	1370						13.508	1.00 32.64	8
				VAL	169	18.090		13.863	1.00 23.55	7
2.5	ATOM	1371			169	19.472	46.011	14.163	1.00 27.27	6
25	ATOM	1372	CB	VAL	169	19.728	45.359	15.523	1.00 28.51	6
	ATOM	1373	CG:	1 VAL	169	21.227	45.133	15.757	1.00 26.42	6
	MOTA	1374		2 VAL	169	19.189	46.160	16.696	1.00 27.97	
	ATOM	1375	c	VAL	169	20.011				6
	ATOM	1376					45.022	13.098	1.00 32.65	6
30				VAL	169	19.332	44.056	12.710	1.00 33.21	В
30	MOTA	1377		GLN	170	21.245	45.196	12.689	0.01 33.85	7
	ATOM	1378	CA	GLN	170	21.966	44.390	11.737	0.01 35.75	6
	MOTA	1379	CB	GLN	170	23.335	44.027	12.362	0.01 36.48	6
	ATOM	1380	CG	GLN	170	24.465	44.012	11.347	0.01 37.54	
	ATOM	1381	CD	GLN	170	25.478				6
35	ATOM	1382					45.110	11.599	0.01 37.91	6
55				GLN	170	25.142	46.186	12.096	0.01 38.17	8
	ATOM	1383	NE2		170	26.735	44.846	11.257	0.01 38.21	7
	ATOM	1384	С	GLN	170	21.355	43.088	11.241	0.01 36.70	6
	ATOM	1385	0	GLN	170	21.049	42.167	11.995	0.01 36.81	8
	ATOM	1386	N	VAL	171	21.273	42.959	9.919	0.01 37.51	7
40	ATOM	1387	CA	VAL	171	20.781				
	ATOM	1388	CB	VAL			41.772	9.240	0.01 38.20	6
					171	19.483	41.208	9.842	0.01 38.61	6
	ATOM	1389		VAL	171	18.334	42.199	9.681	0.01 38.88	6
	ATOM	1390	CG2	VAL	171	19.115	39.881	9.180	0.01 38.83	6
	ATOM	1391	С	VAL	171	20.587	42.048	7.750	0.01 38.42	6
45	ATOM	1392	0	VAL	171	21.420	41.573	6.949	0.01 38.53	8
	ATOM	1393		WAT	201	13.958	68.106			
	MOTA	1394		WAT	202			19.930	1.00 18.36	8
		1395				13.653	41.241	23.320	1.00 24.59	8
	ATOM			WAT	203	5.895	57.410	18.965	1.00 14.14	8
	ATOM	1396	OWO	WAT	204	9.519	72.688	30.514	1.00 42.11	8
50	ATOM	1397	OWO	WAT	205	8.700	64.454	28.355	1.00 21.65	8
	ATOM	1398	OWO	WAT	206	25.548	65.664	7.898	1.00 24.88	8
	ATOM	1399		WAT	207	2.902	52.471			
	ATOM	1400		WAT	208	14.303		31.897	1.00 19.13	8
	ATOM	1401					45.256	23.676	1.00 24.28	8
55				WAT	209	10.371	62.552	29.076	1.00 27.73	8
55	ATOM	1402		WAT	210	12.433	66.629	21.505	1.00 14.04	8
	ATOM	1403	OW0	WAT	211	5.417	47.499	21.002	1.00 16.89	В
	ATOM	1404	OW0	WAT	212	29.599	82.797	11.595	1.00 34.62	8
	ATOM	1405	OWO	WAT	213	17.813	70.187			
	ATOM	1406		WAT	214			2.648	1.00 16.34	8
60						6.656	58.315	16.413	1.00 24.31	8
00	ATOM	1407		WAT	215	21.191	80.146	5.335	1.00 30.05	8
	MOTA	1408		WAT	216	15.621	66.766	18.319	1.00 18.82	8
	ATOM	1409	OW0	WAT	217	6.528	56.410	14.460	1.00 26.68	8
	ATOM	1410		WAT	218	6.213	69.723	22.792	1.00 19.89	
	ATOM	1411		WAT	219	12.935				8
65	ATOM	1412					67.874	24.109	1.00 29.95	8
				WAT	220	-2.277	62.236	20.953	1.00 28.34	8
	ATOM	1413		WAT	221	20.151	71.344	0.183	1.00 21.62	8
	ATOM	1414	OWO		222	27.773	65.203	6.295	1.00 20.74	8
	ATOM	1415	OWO	WAT	223	-0.481	58.864	19.811	1.00 24.67	8
	ATOM	1416	OWO		224	17.815	67.914	1.120	1.00 26.99	
70	ATOM	1417	OWO		225	16.604	64.761			8
-	ATOM	1418						25.523	1.00 18.45	8
	414 VII	T-110	OW0	WAI	226	-0.330	59.580	22.516	1.00 29.01	8

								4 00 40 00	
	ATOM	1419	OWO WAT	227	13.324	40.955	17.129	1.00 40.98 1.00 41.91	8 8
	MOTA	1420	OWO WAT	228	9.214	41.380 82.270	22.450 13.850	1.00 50.03	8
	ATOM	1421	TAW OWO	229 230	20.146 21.707	80.353	12.325	1.00 18.46	8
Е	MOTA	1422 1423	OWO WAT	231	15.403	67.167	25.599	1.00 21.44	8
5	MOTA MOTA	1423	OWO WAT	232	12.703	63.258	30.174	1.00 37.28	8
	ATOM	1425	OWO WAT	233	12.479	61.400	39.250	1.00 23.78	8
	ATOM	1426	OWO WAT	234	13.921	59.460	9.106	1.00 40.49	8 8
	MOTA	1427	OWO WAT	235	7.230	72.381	24.432	1.00 41.81 1.00 17.29	8
10	MOTA	1428	TAW 0WO	236	2.989	58.681	19.344 10.180	1.00 17.23	8
	MOTA	1429	OWO WAT	237	12.865 2.754	75.036 67.991	13.259	1.00 35.75	8
	MOTA	1430	OWO WAT	238 239	17.416	57.608	26.641	1.00 32.09	8
	ATOM	1431	OWO WAT	240	31.068	75.579	10.888	1.00 20.85	8
15	ATOM ATOM	1432 1433	OWO WAT	241	17.725	71.985	21.261	1.00 25.43	8
13	ATOM	1434	OWO WAT	242	32.760	65.251	6.079	1.00 38.04	8
	ATOM	1435	OWO WAT	243	14.079	72.373	25.218	1.00 20.23	8 8
	ATOM	1436	OWO WAT	244	16.644	77.936	-2.315	1.00 34.00 1.00 30.63	8
	ATOM	1437	OWO WAT	245	1.790	62.643	35.518 13.639	1.00 30.03	8
20	ATOM	1438	OWO WAT	246	10.026 11.096	76.840 40.538	24.599	1.00 33.25	8
	ATOM	1439	OWO WAT	247 248	19.457	73.016	-2.970	1.00 36.88	8
	MOTA	1440 1441	OWO WAT	249	18.578	60.108	26.756	1.00 30.86	8
	MOTA MOTA	1442	OWO WAT	250	11.119	78.675	16.190	1.00 37.83	8
25	ATOM	1443	OWO WAT	251	2.583	76.687	28.032	1.00 73.18	8 8
	MOTA	1444	OWO WAT	252	0.243	75.153	22.803	1.00 34.15 1.00 23.17	8
	MOTA	1445	OWO WAT	253	33.328 22.212	82.165 87.081	10.255 5.080	1.00 51.41	8
	MOTA	1446	OWO WAT	254 255	21.393	83.921	11.680	1.00 31.47	8
20	ATOM	1447 1448	OWO WAT	256	37.174	72.382	4.349	1.00 36.66	8
30	ATOM ATOM	1449	OWO WAT	257	23.291	53.950	13.981	1.00 45.02	8
	MOTA	1450	TAW 0WO	258	31.521	80.134	5.404	1.00 28.19	8
	ATOM	1451	OWO WAT	259	11.904	78.169	8.209	1.00 61.39 1.00 45.96	8 8
	ATOM	1452	OWO WAT	260	7.393	36.160 70.954	24.668 23.727	1.00 43.30	8
35	ATOM	1453	OWO WAT	261 262	12.356 33.898	69.078	7.353	1.00 32.96	8
	ATOM	1454 1455	OWO WAT	263	28.502	52.764	25.478	1.00 58.40	8
	MOTA MOTA	1456	OWO WAT	264	23.414	37.810	18.427	1.00 35.16	8
	ATOM	1457	OWO WAT	265	4.792	74.631	16.778	1.00 44.49	8
40	MOTA	1458	OWO WAT	266	28.509	77.721	-1.620	1.00 50.51 1.00 45.74	8
	MOTA	1459	OWO WAT	267	19.685	68.488	-0.712 23.620	1.00 43.74	8
	MOTA	1460	OWO WAT	268	10.899 -1.033	74.487 73.720	20.128	1.00 34.52	8
	MOTA	1461	OWO WAT	269 270	15.215	67.397	0.077	1.00 27.35	8
45	MOTA MOTA	1462 1463	OWO WAT	271	8.748	79.989	16.508	1.00 51.59	8
43	ATOM	1464	OWO WAT	272	22.332	82.314	3.707	1.00 30.25	8
	ATOM	1465	OWO WAT	273	23.373	70.771	17.610	1.00 22.44	8 8
	MOTA	1466	OWO WAT	274	11.965	67.872	26.359 7.198	1.00 26.92 1.00 27.19	8
	MOTA	1467	OWO WAT	275	35.793 10.333	71.146 72.530	25.867	1.00 46.78	8
50	MOTA	1468	OWO WAT	276 277	17.230	69.185	24.852	1.00 26.22	8
	ATOM	1469	OWO WAI	278	17.594	51.432	30.830	1.00 32.58	8
	ATOM ATOM	1470 1471		279	8.561	67.703	32.884	1.00 37.04	8
	ATOM	1472	OWO WAT	280	16.374	71.765	-4.195	1.00 31.45	8
55	ATOM	1473	OWO WAT	281	8.995	70.329	24.946	1.00 36.64 1.00 48.06	8 8
	MOTA	1474	OWO WAT	282	19.019	47.051	28.676	1.00 23.23	8
	MOTA	1475		283	20.039 21.308	61.350 55.309	15.742 20.658	1.00 28.24	8
	ATOM	1476		284 285	7.405	70.019	5.261	1.00 41.47	8
60	MOTA MOTA	1477 1478		286	23.729	66.066	0.632	1.00 30.27	8
60	ATOM	1479		287	15.826	40.095	23.946	1.00 41.94	8
	ATOM	1480		288	-0.119	50.371	24.812	0.50 25.93	8
	MOTA	1481	OWO WAT	289	3.397	54.879	42.245	1.00 29.87 1.00 43.33	8 8
	MOTA	1482		290	10.215	53.151	32.270 33.883	1.00 43.33	8
65	MOTA	1483	OWO WAT	291	8.440	65.109	JJ.00J	1.00 01.00	-
	END								

	nman ny	Total May	20 1 0	:23:51 1998	3				
	CRYST1	79.22	21 100	.866 28.3	172 90.00	90.00	90.00		
	ORIGX1		.000000	0.000000	0.000000		0.00000		
	ORIGX2		.000000	1.000000	0.000000		0.00000		
5	ORIGX3		.000000	0.000000	1.000000		0.00000		
	SCALE1		.012623	0.000000	0.000000		0.00000		
	SCALE2		.000000	0.009914	0.03549		0.00000		
	SCALE3		.000000 CB ALA		36.645	68.826	-4.702	1.00 51.37	6
10	ATOM ATOM		C ALA		36.199	68.294	-2.285	1.00 42.22	6
10	ATOM		O ALA	_	36.801	67.492	-1.569	1.00 42.70	8
	ATOM		N ALA	. 1	34.367	68.121	-3.997	1.00 45.74	7 6
	ATOM	5	CA ALA	_	35.829	67.992	-3.724	1.00 43.68 1.00 40.54	7
	MOTA	_	N PRO	_	35.903	69.499	-1.817 -2.533	1.00 38.91	6
15	MOTA		CD PRO	_	35.149 36.172	70.546 69.844	-0.425	1.00 38.61	6
	ATOM		CA PRO		35.765	71.300	-0.322	1.00 39.86	6
	ATOM		CB PRO	_	34.790	71.513	-1.426	1.00 41.36	6
	ATOM ATOM		C PRO	_	35.294	68.931	0.434	1.00 36.70	6
20	ATOM		O PRO	_	34.188	68.654	-0.042	1.00 32.46	8
20	ATOM		N PRO	_	35.789	68.496	1.579	1.00 33.82	7
	ATOM	14	CD PRO		37.120	68.857	2.110	1.00 35.16 1.00 38.25	6 6
	ATOM		CA PRO		35.069	67.637	2.491 3.799	1.00 37.39	6
	MOTA		CB PRO	_	35.872	67.639 68.267	3.486	1.00 37.41	6
25	MOTA	_	CG PRO	_	37.180 33.653	68.136	2.790	1.00 37.48	6
	ATOM		C PRO	_	33.393	69.335	2.683	1.00 34.39	8
	MOTA		O PRO		32.763	67.212	3.173	1.00 37.04	7
	MOTA MOTA		CA LYS	_	31.399	67.678	3.424	1.00 34.97	6
30	MOTA	22	CB LYS		30.318	66.664	3.122	1.00 43.98	6
00	MOT.		CG LYS		30.564	65.191	3.278	1.00 47.64	6 6
	MOTA	24	CD LYS		29.775	64.349	2.292 2.137	1.00 52.03 1.00 57.56	6
	MOTA	25	CE LYS		28.317 27.72 4	64.743 64.253	0.855	1.00 56.40	7
2.5	MOTA	26	NZ LYS	_	31.243	68.234	4.825	1.00 31.44	6
35	ATOM	27 28	C LYS		31.846	67.769	5.784	1.00 29.91	8
	MOTA MOTA	29	N AL	_	30.416	69.280	4.908	1.00 28.75	7
	ATOM	30	CA ALI	_	30.039	69.813	6.218	1.00 27.21	6
	ATOM	31	CB ALL		29.155	71.032	6.110	1.00 21.94	6 6
40	MOTA	32	C ALJ	_	29.278	68.683	6.923	1.00 26.42 1.00 26.10	8
	MOTA	33	O AL		28.760	67.794 68.674	6.222 8.241	1.00 24.91	7
	MOTA	34	N VA		29.231 28.515	67.632	8.985	1.00 26.95	6
	MOTA	35 36	CA VAL		29.490	66.738	9.770	1.00 29.36	6
45	atom atom	37	CG1 VA		28.779	65.726	10.676	1.00 29.86	6
43	ATOM	38	CG2 VA		30.434	66.024	8.801	1.00 26.74	6
	MOTA	39	C VA		27.503	68.253	9.942	1.00 28.93	6 8
	MOTA	40	O VA	_	27.846	68.994	10.866	1.00 31.46 1.00 30.08	7
	ATOM	41	N LE		26.233 25.105	67.929 68.383	9.758 10.546	1.00 30.00	6
50	MOTA	42	CA LE		23.103	68.346	9.657	1.00 33.18	6
	MOTA	43	CB LE		22.828	69.458	9.960	1.00 34.94	6
	ATOM	44 45	CG LE	_	22.082	69.876	8.721	1.00 27.55	6
	ATOM ATOM	46	CD2 LE		21.887	69.002	11.069	1.00 32.30	6
55	ATOM	47	C LE	_	24.816	67.565	11.794	1.00 29.57	6
	MOTA	48	O LE		24.653	66.351	11.800	1.00 30.04	. 8 . 7
	ATOM	49	N LY		24.768	68.242	12.930	1.00 28.04 1.00 25.12	6
	MOTA	50	CA LY		24.568	67.692	14.257 15.132	1.00 23.12	6
	ATOM	51	CB LY		25.738 25.777	68.179 67.611	16.532	1.00 39.37	6
60	MOTA	52	CG LY	_	25.967	68.598	17.652	1.00 43.84	6
	ATOM	53 54	CE LY	_	27.129	69.561	17.487	1.00 47.78	6
	MOTA MOTA	55	NZ LY	_	27.525	70.175	18.793	1.00 48.98	7
	ATOM	56	C LY	_	23.233	68.192	14.797	1.00 24.53	6
65	ATOM	57	O LY	s 8	22.934	69.384	14.739	1.00 25.35	8
	ATOM	58	N LE		22.423	67.310	15.333	1.00 24.78 1.00 22.07	7 6
	MOTA	59	CA LE		21.080	67.553	15.843 15.190	1.00 22.07	6
	MOTA	60	CB LE	_	20.189 18.725	66.483 66.363	15.190	1.00 20.57	6
70	MOTA	61	CG LE		17.980	67.624	15.214	1.00 19.57	6
70	ATOM	62 63	CD1 LE		18.084	65.137	14.903	1.00 23.44	6
	MOTA	0.5	Hi						

ATOM 67		ATON ATON ATON	65 O LEU	و ا	21.019 67.415 17.346 1.00 21.01 6 21.424 66.393 17.869 1.00 22.38 8
ATOM 68 CB GA GIU 10 21.523 69.162 20.270 1.00 27.36 6 ATOM 70 CGB GIU 10 22.946 68.657 20.195 0.50 28.21 6 ATOM 71 CDB GIU 10 22.946 68.657 20.195 0.50 28.22 6 ATOM 72 CDB GIU 10 23.100 67.202 20.587 0.50 28.25 6 ATOM 73 CDB GIU 10 23.100 67.202 20.587 0.50 24.348 6 ATOM 74 CB GIU 10 23.100 67.202 20.587 0.50 24.348 6 ATOM 75 CB CB GIU 10 23.100 67.202 20.587 0.50 24.348 6 ATOM 76 CB CB GIU 10 23.888 71.008 20.186 0.50 22.108 6.50 22	c	ATOM	67 CA GLU		20 490 60 505 40 4-4
ATOM 70 CCG GLU 10 22.946 68.65.79 20.990 0.50 28.21 6 ATOM 71 CDA GLU 10 23.100 67.202 20.527 0.50 28.55 6 ATOM 73 OEI GLU 10 23.100 67.202 20.527 0.50 28.55 6 ATOM 74 OEI GLU 10 23.100 67.202 20.527 0.50 28.55 6 ATOM 75 OEZ GLU 10 23.888 71.008 20.50 46.42 8 ATOM 77 C G GLU 10 10 19.96 68.728 20.008 1.00 19.76 6 ATOM 79 N GLU 10 11 18.701 69.842 19.613 1.00 18.076 6 ATOM 79 N GLU 10 11 18.701 69.842 19.613 1.00 18.076 6 ATOM 80 CD PRO 11 17.058 68.340 21.390 1.00 18.71 6 ATOM 80 CD PRO 11 10.834 66.62 21.319 1.00 18.46 6 ATOM 80 CD PRO 11 16.550 66.272 22.355 1.00 17.38 6 ATOM 80 CD PRO 11 16.550 66.212 19.81 1.00 18.70 6 ATOM 80 CD PRO 11 18.701 69.842 19.613 1.00 18.06 66.20 21.390 1.00 18.71 69.80 6.50 22.30 6.20 6.20 6.20 6.20 6.20 6.20 6.20 6.2	5				21.523 69.182 20.270 1.00 27.36 6
ATOM 71 CDB GLU 10 24.047 69.789 20.422 20.38.25 5					22 846 68 657
10 ATOM 73 GES GLU 10 23.100 67.202 20.587 0.50 43.48 6 ATOM 74 021 GLU 10 22.443 66.771 21.565 0.50 47.24 8 ATOM 75 02 GLU 10 23.871 10.08 20.186 0.50 22.10 8 ATOM 76 02 GLU 10 23.871 10.08 20.186 0.50 22.10 8 ATOM 77 C GLU 10 23.871 10.08 20.186 0.50 22.10 8 ATOM 78 0 GLU 10 10.936 68.772 21.565 0.50 47.24 8 ATOM 78 0 GLU 10 10.905 68.728 20.008 1.00 19.07 6 ATOM 78 0 GLU 11 10.18.701 69.842 19.5613 1.00 18.07 6 ATOM 79 N PRO 11 17.428 67.395 20.088 1.00 19.07 7 ATOM 80 CD PRO 11 17.807 66.52 21.319 1.00 18.44 6 ATOM 79 N PRO 11 17.807 66.52 21.319 1.00 18.84 6 ATOM 79 N PRO 11 17.807 66.52 21.319 1.00 18.84 6 ATOM 79 N PRO 11 18.834 66.22 21.319 1.00 18.84 6 ATOM 79 N PRO 11 18.300 66.22 21.351 1.00 18.07 6 ATOM 85 0 PRO 11 18.300 66.212 20.365 1.00 17.38 6 ATOM 79 N PRO 12 19.915 63.948 21.361 1.00 18.22 8 ATOM 86 N PRO 12 19.922 64.121 10.00 19.94 7 ATOM 89 CG PRO 12 19.915 63.948 21.361 1.00 19.94 7 ATOM 89 CG PRO 12 19.915 63.948 21.361 1.00 19.94 7 ATOM 90 CG PRO 12 20.292 66.212 10.00 19.94 7 ATOM 90 CG PRO 12 20.292 62.556 19.397 1.00 19.86 6 ATOM 90 CG PRO 12 20.292 62.556 19.397 1.00 19.86 6 ATOM 90 CG PRO 12 20.292 62.556 19.397 1.00 19.86 8 ATOM 90 CG PRO 12 20.292 62.556 19.397 1.00 19.86 8 ATOM 90 CG PRO 12 18.179 63.061 18.395 1.00 18.20 6 ATOM 90 CG PRO 12 18.179 63.061 18.395 1.00 18.20 6 ATOM 90 CG PRO 12 18.266 62.75 12.807 1.00 19.80 6 ATOM 90 CG PRO 12 18.266 62.75 12.807 1.00 19.80 6 ATOM 90 CG PRO 12 18.266 62.75 12.807 1.00 19.80 6 ATOM 90 CG PRO 12 18.266 62.75 12.807 1.00 19.80 6 ATOM 90 CG PRO 12 18.266 62.75 12.807 1.00 19.80 6 ATOM 90 CG PRO 12 18.266 62.75 12.807 1.00 19.80 6 ATOM 90 CG PRO 12 18.266 62.75 12.807 1.00 19.80 6 ATOM 90 CG PRO 12 18.266 62.75 12.807 1.00 19.80 6 ATOM 90 CG PRO 12 18.266 62.75 12.807 1.00 19.80 6 ATOM 90 CG PRO 12 18.266 62.75 12.807 1.00 19.80 6 ATOM 90 CG PRO 12 18.266 62.75 12.807 1.00 19.80 6 ATOM 90 CG PRO 12 18.181 1.00 19.50 6 ATOM 90 CG PRO 12 18.181 1.00 19.50 6 ATOM 90 CG PRO 13 18.266 62.75 18.30 18.30 18.00 19.80 6 ATOM 90 CG PRO 13 18.26				10	24.047 69.789 20.422 0.50 28.55 6
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ATOM 93 N TRP 13 17.039 63.169 19.059 1.00 15.64 7 ATOM 94 CA TRP 13 15.815 62.568 18.561 1.00 17.91 6 ATOM 95 CB TRP 13 15.815 62.568 18.561 1.00 17.91 6 ATOM 96 CG TRP 13 15.815 62.568 18.561 1.00 17.91 6 ATOM 97 CD2 TRP 13 15.633 61.612 21.703 1.00 16.77 6 ATOM 98 CE2 TRP 13 15.633 61.612 21.703 1.00 16.90 6 ATOM 99 CE3 TRP 13 15.867 60.279 21.350 1.00 16.90 6 ATOM 100 CD1 TRP 13 15.106 63.769 21.916 1.00 18.93 6 ATOM 102 CZ2 TRP 13 15.589 63.343 23.137 1.00 11.16 7 ATOM 103 CZ3 TRP 13 15.589 63.343 23.137 1.00 11.16 7 ATOM 104 CH2 TRP 13 16.645 59.825 23.611 1.00 15.92 6 ATOM 105 C TRP 13 15.283 64.238 16.908 1.00 15.92 6 ATOM 105 C TRP 13 15.283 64.238 16.908 1.00 17.22 8 ATOM 106 C TRP 13 15.283 64.238 16.908 1.00 17.22 8 ATOM 107 N LLE 14 15.101 62.078 16.275 1.00 16.57 7 ATOM 110 CG2 LLE 14 15.105 61.521 13.840 1.00 16.57 7 ATOM 111 CG1 LLE 14 15.105 61.521 13.840 1.00 16.67 6 ATOM 111 CG1 LLE 14 15.466 62.441 14.936 1.00 16.67 6 ATOM 112 CD1 LLE 14 15.045 59.150 12.896 1.00 16.67 6 ATOM 113 C LLE 14 15.045 59.150 12.896 1.00 16.67 6 ATOM 114 O LLE 14 15.045 59.955 17.27 1.00 13.35 6 ATOM 115 N ASN 15 10.935 62.270 15.778 1.00 13.35 6 ATOM 124 C ASN 15 10.591 59.946 16.762 1.00 19.46 7 ATOM 124 C ASN 15 10.632 63.124 17.005 1.00 10.15 7 6 ATOM 124 C ASN 15 10.632 63.124 17.005 1.00 10.15 7 6 ATOM 124 C ASN 15 10.666 63.745 18.111 1.00 13.35 8 ATOM 124 C ASN 15 10.666 63.745 18.111 1.00 13.35 8 ATOM 124 C ASN					18.179 63.061 18.395 1.00 18.70 6
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	70										
		ATOM		CB							

	ATOM	206	SG	CYS	26	27.138	73.358	8.311	1.00 22.25	16
	ATOM	207	N	GLN	27	28.929	71.729	11.355	1.00 19.35	7
	ATOM	208	CA	GLN	27	30.332	71.521	11.658	1.00 23.30	6
	ATOM	209	CB	GLN	27	30.543	70.209	12.464	1.00 29.78	6
5	MOTA	210	CG	GLN	27	29.623	70.044	13.672	1.00 31.50	6
	MOTA	211	CD	GLN	27	29.927	68.828	14.518	1.00 33.01	6
	MOTA	212		GLN	27	30.322	67.774	14.032	1.00 38.67	8
	MOTA	213		GLN	27	29.792	68.895	15.834	1.00 36.36	7
	MOTA	214	С	GLN	27	31.169	71.417	10.377	1.00 26.33	6
10	MOTA	215	0	GLN	27	30.764	70.856	9.347	1.00 23.15	8
	MOTA	216	N	GLY	28	32.363	72.019	10.438	1.00 27.69	7
	ATOM	217	CA	GLY	28	33.289	72.019 73.360	9.313	1.00 28.02 1.00 29.41	6 6
	ATOM	218	C	GLY	28 28	34.022 33.639	74.335	9.215 9.862	1.00 29.41	8
15	ATOM	219 220	O N	GLY ALA	29	35.062	73.421	8.389	1.00 27.48	7
10	ATOM ATOM	221	CA	ALA	29	35.824	74.640	8.210	1.00 27.39	6
	ATOM	222	CB	ALA	29	36.979	74.353	7.239	1.00 25.91	6
	MOTA	223	C	ALA	29	34.959	75.730	7.574	1.00 28.27	6
	ATOM	224	ŏ	ALA	29	34.315	75.415	6.561	1.00 26.07	8
20	ATOM	225	N	ARG	30	35.060	76.951	8.064	1.00 23.97	7
20	ATOM	226	CA	ARG	30	34.303	78.055	7.490	1.00 27.17	6
	ATOM	227	CB	ARG	30	33.571	78.823	8.601	1.00 30.34	6
	ATOM	228	CG	ARG	30	32.574	78.090	9.460	1.00 34.05	6
	ATOM	229	CD	ARG	30	32.365	78.880	10.761	1.00 33.86	6
25	ATOM	230	NE	ARG	30	32.407	77.902	11.836	1.00 38.60	7
	ATOM	231	CZ	ARG	30	32.487	78.082	13.126	1.00 38.08	6
	ATOM	232	NH1	ARG	30	32.567	79.298	13.635	1.00 36.51	7
	ATOM	233	NH2	ARG	30	32.467	76.990	13.879	1.00 46.13	7
••	ATOM	234	С	ARG	30	35.194	79.148	6.880	1.00 26.70	6
30	ATOM	235	0	ARG	30	36.399	79.142	7.075	1.00 29.22	8
	ATOM	236	N	SER	31	34.573	80.129	6.246	1.00 26.85	7
	ATOM	237	CA	SER	31	35.315	81.284	5.738	1.00 26.56 1.00 25.03	6 6
	MOTA	238	CB OG	SER SER	31 31	34.682 34.562	81.846 80.875	4.476 3.477	1.00 23.03	8
35	MOTA MOTA	239 240	C	SER	31	35.273	82.321	6.861	1.00 26.58	6
33	ATOM	241	ŏ	SER	31	34.396	82.246	7.739	1.00 23.91	8
	ATOM	242	N	PRO	32	36.163	83.308	6.839	1.00 23.48	7
	ATOM	243	CD	PRO	32	37.224	83.483	5.842	1.00 22.70	6
	MOTA	244	CA	PRO	32	36.176	84.350	7.861	1.00 24.75	6
40	ATOM	245	CB	PRO	32	37.621	84.830	7.805	1.00 24.34	6
	MOTA	246	CG	PRO	32	38.095	84.571	6.414	1.00 23.77	6
	MOTA	247	C	PRO	32	35.172	85.449	7.549	1.00 29.23	6
	ATOM	248	0	PRO	32	35.472	86.609	7.223 7.709	1.00 28.28 1.00 29.77	8 7
45	ATOM ATOM	249 250	N CA	GLU GLU	33 33	33.913 32.725	85.121 85.896	7.417	1.00 23.77	6
40	ATOM	251		GLU	33	32.177	85.426	6.073	0.50 35.18	6
	ATOM	252		GLU	33	32.123	85.457	6.084	0.50 31.98	6
	ATOM	253		GLU	33	30.795	84.829	5.952	0.50 39.40	6
	ATOM	254		GLU	33	31.776	83.990	5.954	0.50 34.05	6
50	ATOM	255		GLU	33	30.394	84.525	4.521	0.50 46.48	6
	ATOM	256	CDB	GLU	33	31.601	83.533	4.517	0.50 34.67	6
	ATOM	257	OE1	GLU	33	29.268	84.856	4.076		8
	MOTA	258	OE1	GLU	33	32.194	84.168	3.619	0.50 32.81	8
	MOTA	259		GLU	33	31.232	83.952	3.788	0.50 47.50	8
55	MOTA	260	OE2	GLU	33	30.877	82.542	4.275	0.50 24.64	8
	MOTA	261	С	GLU	33	31.683	85.689	8.519	1.00 32.61	6
	ATOM	262	0	GLU	33	31.612	84.600	9.085	1.00 28.72	8
	MOTA	263	N	SER	34	30.844	86.682	8.743	1.00 32.15	7
60	MOTA	264	CA	SER SER	34 34	29.804 29.277	86.591 88.013	9.764 10.037	1.00 32.72 1.00 34.26	6 6
00	MOTA MOTA	265 266	CB OG	SER	34	28.320	87.931	11.093	1.00 45.88	8
	ATOM	267	c	SER	34	28.668	85.674	9.332	1.00 30.93	6
	ATOM	268	ŏ	SER	34	28.156	84.883	10.124	1.00 28.87	8
	ATOM	269	N	ASP	35	28.222	85.773	8.082	1.00 28.02	7
65	ATOM	270	CA	ASP	35	27.167	84.858	7.599	1.00 28.62	6
	ATOM	271	CB	ASP	35	26.292	85.538	6.585	1.00 29.65	6
	ATOM	272	CG	ASP	35	25.357	86.639	7.057	1.00 37.43	6
	MOTA	273		ASP	35	25.027	86.769	8.258	1.00 33.53	8
70	MOTA	274		ASP	35 35	24.902	87.396	6.154	1.00 36.01	8
70	MOTA	275	C	ASP	35 35	27.882	83.643	6.973	1.00 27.08	6
	MOTA	276	0	ASP	35	27.997	83.566	5.756	1.00 28.07	8

	MOTA	277 N SER	36	28.461 82.74	3 7.774 1.00 25.55 7
	ATOM	278 CA SER	36	29.282 81.68	,
	MOTA	279 CB SER	36	30.440 81.43	8.213 1.00 34.87 6
5	MOTA MOTA	280 OG SER 281 C SER	36 36	29.973 80.80	
Ü	MOTA	282 O SER	36 36	28.558 80.38; 29.143 79.42;	
	MOTA	283 N ILE	37	27.293 80.223	
	MOTA	284 CA ILE	37	26.580 78.97	
1.0	ATOM	285 CB ILE	37	26.164 78.30	
10	ATOM	286 CG2 ILE	37	25.561 76.931	8.032 1.00 26.94 6
	ATOM ATOM	287 CG1 ILE 288 CD1 ILE	37 37	27.333 78.221	
	ATOM	289 C ILE	37	28.443 77.278 25.336 79.159	
4 -	ATOM	290 O ILE	37	24.515 80.033	
15	ATOM	291 N GLN	38	25.122 78.314	
	MOTA	292 CA GLN	38	23.862 78.296	4.399 1.00 23.13 6
	MOTA MOTA	293 CB GLN 294 CG GLN	38 38	24.016 78.068	
	ATOM	295 CD GLN	38	24.458 79.296 24.692 78.965	
20	ATOM	296 OE1 GLN	38	25.540 78.122	
	ATOM	297 NE2 GLN	38	23.922 79.668	
	MOTA	298 C GLN	38	23.048 77.128	4.985 1.00 23.81 6
	ATOM ATOM	299 O GLN 300 N TRP	38	23.598 76.022	5.087 1.00 22.62 B
25	ATOM	300 N TRP 301 CA TRP	39 39	21.807 77.386 20.987 76.304	,
	MOTA	302 CB TRP	39	20.345 76.633	5.905 1.00 21.73 6 7.257 1.00 21.01 6
	ATOM	303 CG TRP	39	21.264 76.633	8.430 1.00 17.58 6
	ATOM	304 CD2 TRP	39	21.721 75.523	9.212 1.00 17.00 6
30	ATOM ATOM	305 CE2 TRP 306 CE3 TRP	39 39	22.569 76.033	10.220 1.00 16.71 6
	ATOM	307 CD1 TRP	39	21.495 74.147 21.844 77.750	9.158 1.00 21.47 6
	ATOM	308 NEI TRP	39	22.626 77.400	8.974 1.00 19.92 6 10.061 1.00 22.18 7
	MOTA	309 CZ2 TRP	39	23.218 75.220	11.152 1.00 18.29 6
35	ATOM	310 CZ3 TRP	39	22.109 73.329	10.091 1.00 21.62 6
33	ATOM ATOM	311 CH2 TRP 312 C TRP	39 30	22.960 73.874	11.064 1.00 20.15 6
	ATOM	312 C TRP 313 O TRP	39 39	19.890 75.993 19.407 76.925	4.898 1.00 22.76 6
	ATOM	314 N PHE	40	19.407 76.925 19.533 74.701	4.238 1.00 23.42 8 4.758 1.00 22.91 7
40	ATOM	315 CA PHE	40	18.512 74.389	3.754 1.00 26.86 6
40	ATOM	316 CB PHE	40	19.121 73.722	2.513 1.00 24.16 6
	ATOM ATOM	317 CG PHE 318 CD1 PHE	40	20.225 74.429	1.788 1.00 23.96 6
	ATOM	318 CD1 PHE 319 CD2 PHE	40 40	21.551 74.280 19.945 75.244	2.189 1.00 23.61 6
4 =	ATOM	320 CE1 PHE	40	22.564 74.919	0.696 1.00 22.47 6 1.504 1.00 20.83 6
45	ATOM	321 CE2 PHE	40	20.967 75.880	0.020 1.00 21.69 6
	ATOM	322 CZ PHE	40	22.267 75.740	0.432 1.00 21.86 6
	ATOM ATOM	323 C PHE 324 O PHE	40 40	17.466 73.435	4.349 1.00 23.51 6
	ATOM	325 N HIS	41	17.838 72.588 16.232 73.575	5.151 1.00 21.94 8 3.905 1.00 21.59 7
50	ATOM	326 CA HIS	41	15.107 72.771	3.905 1.00 21.59 7 4.366 1.00 24.07 6
	ATOM	327 CB HIS	41	14.032 73.572	5.099 1.00 18.72 6
	ATOM ATOM	328 CG HIS	41	12.864 72.727	5.548 1.00 23.41 6
	ATOM	329 CD2 HIS 330 ND1 HIS	41 41	12.794 71.415	5.899 1.00 21.85 6
55	ATOM	331 CE1 HIS	41	11.588 73.218 10.789 72.259	5.709 1.00 21.97 7 6.135 1.00 22.79 6
	ATOM	332 NE2 HIS	41	11.504 71.161	6.135 1.00 22.79 6 6.268 1.00 21.87 7
	ATOM	333 C HIS	41	14.455 72.163	3.115 1.00 21.83 6
	ATOM ATOM	334 O HIS 335 N ASN	41	13.972 72.919	2.282 1.00 21.37 8
60	ATOM	335 n asn 336 ca asn	42 42	14.576 70.847	2.959 1.00 22.08 7
	ATOM	337 CB ASN	42	14.077 70.196 12.562 70.322	1.726 1.00 20.46 6
	ATOM	338 CG ASN	42	11.925 69.397	1.722 1.00 18.21 6 2.761 1.00 22.74 6
	ATOM	339 OD1 ASN	42	12.473 68.343	3.087 1.00 24.40 8
65	ATOM	340 ND2 ASN	42	10.804 69.804	3.341 1.00 18.43 7
0.5	ATOM ATOM	341 C ASN	42	14.733 70.811	0.488 1.00 21.32 6
	ATOM	342 O ASN 343 N GLY	42 43	14.085 71.047	-0.533 1.00 20.13 8
	ATOM	344 CA GLY	43	16.002 71.220 16.767 71.861	0.568 1.00 20.53 7
7.0	ATOM	345 C GLY	43	16.586 73.360	-0.480 1.00 20.83 6 -0.661 1.00 24.51 6
70	ATOM	346 O GLY	43	17.209 73.987	-1.550 1.00 25.30 8
	ATOM	347 N ASN	44	15.633 73.970	0.051 1.00 21.27 7

	ATOM ATOM	348 349	CA ASN CB ASN	44 44	15.391 13.903				6
	ATOM	350	CG ASN	44	13.049				6 6
	ATOM	351	OD1 ASN	44	12.148				8
5	ATOM	352	ND2 ASN	44	13.382				7
	ATOM	353	C ASN	44	16.208				6
	ATOM ATOM	354 355	O ASN N LEU	44 45	16.180				8
	ATOM	356	CA LEU	45	16.907 17.730				7
10	ATOM	357	CB LEU	45	18.391				6 6
	ATOM	358	CG LEU	45	19.159				6
	MOTA	359	CD1 LEU	45	20.479	79.571	2.002		6
	MOTA		CD2 LEU	45	19.452				6
15	MOTA ATOM		C LEU	45 45	16.825	78.559		1.00 22.27	6
10	ATOM		N ILE	46	15.748 17.263	78.997 78.604		1.00 20.13 1.00 20.11	8 7
	ATOM		CA ILE	46	16.539	79.322		1.00 24.64	6
	ATOM		CB ILE	46	16.657	78.508		1.00 22.24	6
20	ATOM		CG2 ILE	46	16.007	79.134		1.00 21.33	6
20	ATOM		CG1 ILE	46	16.111	77.072		1.00 20.74	6
	ATOM ATOM		CD1 ILE C ILE	46 46	16.664 17.351	76.147		1.00 20.48	6
	ATOM		O ILE	46	18.419	80.625 80.600	5.006 5.624	1.00 25.53 1.00 22.91	6 8
	ATOM		N PRO	47	16.937	81.747	4.444	1.00 22.91	7
25	ATOM		CD PRO	47	15.704	81.884	3.620	1.00 32.61	6
	ATOM		CA PRO	47	17.731	82.968	4.434	1.00 30.93	6
	ATOM ATOM		CB PRO	47 47	17.030	83.836	3.363	1.00 31.28	6
	ATOM		C PRO	47	15.610 17.888	83.400 83.762	3.441 5.706	1.00 32.54	6
30	ATOM		O PRO	47	18.733	84.670	5.747	1.00 28.32 1.00 29.24	6 8
	ATOM		N THR	48	17.092	83.513	6.730	1.00 26.79	7
	ATOM		CA THR	48	17.135	84.298	7.971	1.00 26.97	6
	ATOM ATOM		CB THR OG1 THR	48	15.698	84.323	8.532	1.00 31.78	6
35	ATOM		CG2 THR	48 48	15.241 14.798	82.958 85.150	8.520 7.605	1.00 31.45	8
	ATOM		THR	48	18.075	83.757	9.021	1.00 27.40 1.00 26.31	6 6
	ATOM		O THR	48	18.206	84.334	10.113	1.00 28.00	8
	MOTA		N HIS	49	18.698	82.602	8.772	1.00 24.44	7
40	MOTA		LA HIS	49	19.612	81.942	9.707	1.00 24.19	6
40	ATOM ATOM		CB HIS	49 49	18.953	80.610	10.174	1.00 25.11	6
	ATOM		D2 HIS	49	17.722 16.430	80.939 81.109	10.961 10.624	1.00 22.20 1.00 27.86	6
	ATOM		D1 HIS	49	17.809	81.225	12.306	1.00 27.86	6 7
4.5	ATOM		E1 HIS	49	16.595	81.526	12.762	1.00 28.91	6
45	ATOM		TE2 HIS	49	15.748	81.474	11.761	1.00 25.35	7
	ATOM ATOM	393 C		49	20.923	81.588	9.041	1.00 23.08	6
	ATOM	394 C		49 50	20.942 22.038	80.805 82.162	8.075	1.00 20.57	8
	ATOM		A THR	50	23.321	81.974	9.497 8.807	1.00 25.11 1.00 22.98	7 6
50	ATOM		B THR	50	23.732	83.314	8.137	1.00 23.01	6
	ATOM		G1 THR	50	23.843	84.252	9.231	1.00 18.66	8
	MOTA		G2 THR	50	22.757	83.817	7.101	1.00 19.07	6
	ATOM ATOM	400 C		50 50	24.460 25.640	81.645	9.766	1.00 24.61	6
55	ATOM	402 N		51	24.126	81.772 81.274	9.393 10.985	1.00 26.17 1.00 24.52	8 7
	ATOM		A GLN	51	25.132	80.979	11.995	1.00 27.31	6
	ATOM	404 C		51	24.708	81.505	13.378	1.00 28.63	6
	ATOM	405 C		51	24.438	83.014	13.378	1.00 32.81	6
60	ATOM ATOM	406 C		51 51	25.677	83.810	12.995	1.00 38.53	6
	ATOM		E1 GLN E2 GLN	51 51	26.606 25.724	83.952 84.331	13.802 11.765	1.00 37.60 1.00 32.79	8
	ATOM	409 C		51	25.411	79.487	12.101	1.00 32.79	7 6
	MOTA	4 10 0		51	24.626	78.636	11.689	1.00 26.27	8
C.F.	ATOM	411 N		52	26.510	79.138	12.769	1.00 25.16	7
65	ATOM	412 CI		52	27.553	80.091	13.270	1.00 24.54	6
	ATOM ATOM	413 CI 414 CI		52 52	26.917 28.264	77.763	12.974	1.00 25.24	6
	ATOM	415 C		52	28.264 28.804	77.888 79.217	13.708 13.257	1.00 26.09 1.00 23.35	6 6
	ATOM	416 C	PRO	52	25.900	76.915	13.722	1.00 25.71	6
70	ATOM	417 0	PRO	52	25.877	75.687	13.542	1.00 21.61	8
	MOTA	418 N	SER	53	25.044	77.497	14.556	1.00 24.05	7

	ATOM	419 CA SER	53	23.991 76.773 15.239 1.00 25.63	3 6
	MOTA MOTA	420 CB SER 421 OG SER	53 53	24.105 76.711 16.758 1.00 31.86	6
	ATOM	422 C SER	53 53	24.778 75.495 17.094 1.00 42.46 22.681 77.460 14.854 1.00 24.85	-
5	ATOM	423 O SER	53	22.681 77.460 14.854 1.00 24.85 22.681 78.673 14.691 1.00 23.68	
	MOTA	424 N TYR	54	21.658 76.689 14.614 1.00 24.52	
	MOTA	425 CA TYR	54	20.333 77.167 14.212 1.00 26.29	
	ATOM ATOM	426 CB TYR 427 CG TYR	54 54	20.050 76.886 12.729 1.00 26.92	
10	ATOM	428 CD1 TYR	54	18.612 76.998 12.274 1.00 30.15 17.719 77.905 12.825 1.00 29.18	
	ATOM	429 CE1 TYR	54	17.719 77.905 12.825 1.00 29.18 16.407 78.006 12.409 1.00 31.26	-
	ATOM	430 CD2 TYR	54	18.104 76.166 11.280 1.00 31.67	
	ATOM ATOM	431 CE2 TYR 432 CZ TYR	54	16.796 76.217 10.855 1.00 31.66	6
15	ATOM	432 CZ TYR 433 OH TYR	54 54	15.950 77.151 11.429 1.00 33.63 14.624 77.219 11.038 1.00 34.53	_
	ATOM	434 C TYR	54	14.624 77.219 11.038 1.00 34.53 19.378 76.450 15.167 1.00 24.84	
	MOTA	435 O TYR	54	19.300 75.210 15.129 1.00 22.53	6 8
	ATOM	436 N ARG	55	18.773 77.181 16.070 1.00 21.66	7
20	MOTA MOTA	437 CA ARG 438 CB ARG	55	17.864 76.650 17.070 1.00 23.60	6
20	MOTA	438 CB ARG 439 CG ARG	55 55	18.242 77.157 18.480 1.00 25.95 17.478 76.340 19.551 1.00 23.98	6
	ATOM	440 CD ARG	55	17 651	6
	ATOM	441 NE ARG	55	17.651 76.982 20.918 1.00 35.38 16.821 76.365 21.956 1.00 27.47	6 7
25	ATOM	442 CZ ARG	55	17.278 75.530 22.879 1.00 33.10	6
25	ATOM	443 NH1 ARG	55	18.570 75.209 22.904 1.00 30.00	7
	atom Atom	444 NH2 ARG 445 C ARG	55 55	16.418 75.049 23.778 1.00 32.66	7
	ATOM	446 O ARG	55 55	16.434 77.103 16.802 1.00 27.49 16.275 78.312 16.569 1.00 22.62	6
	ATOM	447 N PHE	56	16.275 78.312 16.569 1.00 22.62 15.455 76.174 16.781 1.00 23.78	8 7
30	ATOM	448 CA PHE	56	14.092 76.636 16.510 1.00 21.92	6
	ATOM	449 CB PHE	56	13.716 76.495 15.036 1.00 25.99	6
	atom Atom	450 CG PHE 451 CD1 PHE	56	13.819 75.131 14.386 1.00 20.84	6
	ATOM	451 CD1 PHE 452 CD2 PHE	56 56	15.019 74.653 13.897 1.00 21.33 12.705 74.319 14.264 1.00 20.31	6
35	ATOM	453 CE1 PHE	56	75 400	6
	MOTA	454 CE2 PHE	56	15.103 /3.415 13.283 1.00 21.52 12.768 73.077 13.680 1.00 18.36	6 6
	ATOM	455 CZ PHE	56	13.973 72.616 13.159 1.00 18.38	6
	ATOM ATOM	456 C PHE	56	13.095 75.862 17.372 1.00 23.93	6
40	ATOM	457 O PHE 458 N LYS	56 57	13.454 74.833 17.921 1.00 22.42	8
	ATOM	459 CA LYS	5 <i>7</i>	11.865 76.340 17.423 1.00 22.46 10.735 75.659 18.054 1.00 24.34	7
	ATOM	460 CBA LYS	57	9.892 76.620 18.881 0.50 28.51	6 6
	ATOM	461 CBB LYS	57	9.822 76.727 18.669 0.50 22.87	6
45	ATOM ATOM	462 CGA LYS 463 CGB LYS	57	10.656 77.298 20.010 0.50 33.64	6
10	ATOM	463 CGB LYS 464 CDA LYS	57 57	8.769 76.208 19.632 0.50 24.29 11.436 76.342 20.892 0.50 40.75	6
	ATOM	465 CDB LYS	57	11.436 76.342 20.892 0.50 40.75 8.631 77.186 20.798 0.50 26.90	6
	ATOM	466 CEA LYS	57	12.612 76.990 21.603 0.50 43.07	6 6
ΕΛ	ATOM	467 CEB LYS	57	9.138 76.604 22.092 0.50 29.79	6
50	ATOM	468 NZA LYS	57	12.703 76.630 23.044 0.50 51.71	7
	ATOM ATOM	469 NZB LYS 470 C LYS	57 57	8.050 76.265 23.060 0.50 36.22	7
	ATOM	471 O LYS	57 57	9.950 74.923 16.969 1.00 21.30 9.436 75.551 16.052 1.00 19.46	6
	MOTA	472 N ALA	58	9.436 75.551 16.052 1.00 19.46 9.928 73.588 16.945 1.00 18.23	8 7
55	MOTA	473 CA ALA	58	9.341 72.864 15.821 1.00 15.74	6
	ATOM	474 CB ALA	58	9.612 71.361 16.094 1.00 9.09	6
	MOTA MOTA	475 C ALA 476 O ALA	58	7.841 73.034 15.614 1.00 20.26	6
	ATOM	476 O ALA 477 N ASN	58 59	7.067 73.064 16.574 1.00 18.04	8
60	ATOM	478 CA ASN	59	7.392 73.126 14.367 1.00 18.31 5.986 73.071 14.019 1.00 23.04	7
	MOTA	479 CB ASN	59	5.986 73.071 14.019 1.00 23.04 5.222 74.301 13.612 1.00 32.39	6 6
	MOTA	480 CG ASN	59	5.880 75.643 13.665 1.00 38.26	6
	ATOM	481 OD1 ASN	59	5.855 76.279 14.716 1.00 42.50	8
65	ATOM ATOM	482 ND2 ASN 483 C ASN	59	6.426 76.066 12.529 1.00 43.39	7
	ATOM	483 C ASN 484 O ASN	59 59	5.825 72.052 12.867 1.00 24.07 6.794 71.476 12.365 1.00 21.25	6
	ATOM	485 N ASN	60		8
	MOTA	486 CA ASN	60	4.582 71.833 12.484 1.00 24.40 4.192 70.823 11.519 1.00 31.47	7 6
70	ATOM	487 CB ASN	60	2.680 70.893 11.234 1.00 31.46	6
70	ATOM	488 CGA ASN	60	2.272 69.776 10.274 0.50 31.26	6
	ATOM	489 CGB ASN	60	2.221 72.272 10.814 0.50 35.72	6

	ATOM	490		ASN	60	2.337	68.582	10.597	0.50 22.52	8
	MOTA	491	OD1	ASN	60	2.985	73.240	10.768	0.50 33.04	8
	MOTA	492		ASN	60	1.863	70.175	9.070	0.50 26.04	7
_	ATOM	493	ND2	asn	60	0.932	72.391	10.483	0.50 39.47	7
5	MOTA	494	С	ASN	60	5.006	70.943	10.234	1.00 29.05	6
	MOTA	495	0	asn	60	5.645	69.986	9.780	1.00 32.27	8
	MOTA	496	N	ASN	61	5.098	72.153	9.710	1.00 30.20	7
	ATOM	497		ASN	61	5.863	72.487	8.529	0.50 28.68	6
• •	ATOM	498		ASN	61	5.857	72.367	8.477	0.50 29.13	6
10	MOTA	499		ASN	61	5.564	73.955	8.150	0.50 26.19	6
	ATOM	500		ASN	61	5.403	73.671	7.806	0.50 30.25	6
	ATOM	501		ASN	61	4.101	74.127	7.792	0.50 27.01	6
	ATOM	502		ASN	61	5.608	74.882	8.678	0.50 32.36	6
1 5	ATOM	503		ASN	61	3.502	75.125	8.184	0.50 28.58	8
15	MOTA	504		ASN	61	6.383	74.820	9.637	0.50 33.38	8
	ATOM	505		ASN	61	3.526	73.172	7.071	0.50 34.39	7
	ATOM	506		ASN	61	4.927	75.991	8.384	0.50 33.52	7
	ATOM	507	C	ASN	61	7.371	72.336	8.628	1.00 25.33	6
20	ATOM	508	0	ASN	61 62	8.030 7.932	72.535 71.978	7.617	1.00 21.46	8
20	ATOM	509 510	N CA	ASP ASP	62	9.373	71.842	9.767 9.941	1.00 24.89 1.00 21.37	7 6
	ATOM	511	CB	ASP	62	9.749	72.284	11.372	1.00 21.37	6
	MOTA MOTA	512	CG	ASP	62	9.620	73.782	11.538	1.00 26.20	6
	ATOM	513		ASP	62	9.824	74.549	10.570	1.00 20.20	8
25	ATOM	514		ASP	62	9.276	74.273	12.611	1.00 20.81	8
25	ATOM	515	C	ASP	62	9.887	70.439	9.645	1.00 17.90	6
	ATOM	516	ŏ	ASP	62	11.104	70.209	9.654	1.00 20.50	8
	ATOM	517	N	SER	63	9.011	69.477	9.394	1.00 19.81	7
	ATOM	518	CA	SER	63	9.434	68.132	9.015	1.00 19.84	6
30	ATOM	519	CB	SER	63	8.268	67.164	8.811	1.00 22.04	6
50	ATOM	520	OG	SER	63	7.506	67.018	10.009	1.00 20.02	8
	ATOM	521	c	SER	63	10.196	68.204	7.682	1.00 23.89	6
	ATOM	522	ō	SER	63	10.015	69.160	6.911	1.00 17.92	8
	ATOM	523	N	GLY	64	11.056	67.195	7.467	1.00 19.50	7
35	ATOM	524	CA	GLY	64	11.769	67.191	6.190	1.00 22.23	6
-	ATOM	525	c c	GLY	64	13.272	66.965	6.340	1.00 19.81	6
	ATOM	526	ō	GLY	64	13.744	66.564	7.399	1.00 18.93	8
	ATOM	527	N	GLU	65	13.980	67.226	5.238	1.00 17.01	7
	ATOM	528	CA	GLU	65	15.428	67.013	5.269	1.00 21.39	6
40	ATOM	529		GLU	65	15.934	66.562	3.901	0.50 13.64	6
	ATOM	530	CBB	GLU	65	15.933	66.446	3.947	0.50 23.81	6
	ATOM	531	CGA	GLU	65	16.507	65.158	3.813	0.50 15.71	6
	ATOM	532	CGB	GLU	65	15.409	65.059	3.602	0.50 32.15	6
	MOTA	533	CDA	GLU	65	16.656	64.679	2.381	0.50 22.33	6
45	ATOM	534	CDB	GLU	65	15.898	63.965	4.520	0.50 40.56	6
	ATOM	535	OE1	GLU	65	17.428	65.263	1.586	0.50 22.70	8
	ATOM	536	OE1	GLU	65	16.578	64.271	5.525	0.50 41.83	8
	ATOM	537		GLU	65	15.991	63.686	2.014	0.50 31.04	8
	ATOM	538		GLU	65	15.624	62.758	4.278	0.50 46.02	8
50	ATOM	539	С	GLU	65	16.155	68.324	5.593	1.00 21.56	6
	ATOM	540	0	GLU	65	15.756	69.325	5.007	1.00 21.41	8
	MOTA	541	N	TYR	66	17.172	68.268	6.458	1.00 21.38	7
	ATOM	542	CA	TYR	66	17.966	69.483	6.691	1.00 17.91	6
	atom	543	CB	TYR	66	17.954	69.984	8.129	1.00 17.39	6
55	MOTA	544	CG	TYR	66	16.620	70.563	8.534	1.00 18.08	6
	ATOM	545		TYR	66	15.605	69.686	8.957	1.00 18.56	6
	ATOM	546	CE1		66	14.369	70.147	9.323	1.00 16.48	6
	ATOM	547	CD2	TYR	66	16.348	71.921	8.485	1.00 18.23	6
	ATOM	548		TYR	6 6	15.102	72.382	8.867	1.00 18.37	6
60	ATOM	549	CZ	TYR	66	14.124	71.516	9.279	1.00 18.98	6
	ATOM	550	OH	TYR	66	12.872	71.939	9.624	1.00 14.14	8
	ATOM	551	С	TYR	66	19.379	69.231	6.212	1.00 13.96	6
	ATOM	552	0	TYR	66	19.923	68.135	6.353	1.00 18.14	8
c =	ATOM	553	N	THR	67	20.010	70.228	5.568	1.00 17.95	7
65	ATOM	554	CA	THR	67	21.374	70.138	5.117	1.00 18.06	6
	ATOM	555	CB	THR	67	21.514	69.844	3.599	1.00 22.52	6
	ATOM	556	OG1		67	20.669	70.737	2.835	1.00 16.85	8
	ATOM	557		THR	67	21.215	68.371	3.309	1.00 17.46	6
7.0	ATOM	558	С	THR	67	22.044	71.508	5.384	1.00 18.76	6
70	ATOM	559	0	THR	67	21.354	72.515	5.567	1.00 17.47	8
	MOTA	560	N	CYS	68	23.354	71.540	5.389	1.00 19.74	7

	ATOM	632 CA PRO	78	20.849	65.130	5.098	1.00 25.42	6
	ATOM	633 CB PRO	78	19.795	64.592			6
	ATOM	634 CG PRO	78	20.453	63.586			
	MOTA	635 C PRO	78	20.575			-	6
5	ATOM	636 O PRO	78		64.556			6
Ŭ	ATOM	637 N VAL	79	21.006	63.459			8
				19.833	65.331			7
	ATOM	638 CA VAL	79	19.287	64.861			6
	ATOM	639 CB VAL	79	19.850	65.516		1.00 19.49	6
10	MOTA	640 CG1 VAL	79	19.042	65.239	11.046	1.00 22.25	6
10	MOTA	641 CG2 VAL	79	21.275	64.959	10.036	1.00 21.95	6
	MOTA	642 C VAL	79	17.777	65.046	8.399	1.00 19.76	6
	MOTA	643 O VAL	79	17.283	66.130	8.076	1.00 22.34	8
	ATOM	644 N HIS	80	17.024	63.955	8.566		7
	MOTA	645 CA HIS	80	15.584	63.976	8.387		6
15	MOTA	646 CB HIS	80	15.130	62.621	7.784		6
	ATOM	647 CG HIS	80	13.712	62.754	7.293	1.00 31.93	6
	ATOM	648 CD2 HIS	80	13.194	62.983			
	ATOM	649 ND1 HIS	80	12.637		6.069	1.00 27.05	6
	ATOM	650 CE1 HIS	80		62.697	8.176	1.00 34.35	7
20				11.525	62.847	7.480	1.00 34.80	6
20	ATOM	651 NE2 HIS	80	11.831	63.016	6.210	1.00 34.81	7
	ATOM	652 C HIS	80	14.865	64.187	9.718	1.00 23.08	6
	ATOM	653 O HIS	80	15.096	63.496	10.709	1.00 23.37	8
	ATOM	654 N LEU	81	13.953	65.138	9.747	1.00 19.18	7
	ATOM	655 CA LEU	81	13.244	65.478	10.957	1.00 21.58	6
25	MOTA	656 CB LEU	81	13.567	66.937	11.331	1.00 18.20	6
	MOTA	657 CG LEU	81	12.847	67.381	12.605	1.00 18.21	6
	ATOM	658 CD1 LEU	81	13.496	66.708	13.812	1.00 19.39	
	ATOM	659 CD2 LEU	81	12.865	68.912	12.696		6
	ATOM	660 C LEU	81	11.747			1.00 14.76	6
30	ATOM	661 O LEU	81		65.255	10.783	1.00 19.36	6
	ATOM	662 N THR		11.225	65.543	9.720	1.00 20.96	8
	ATOM		82	11.100	64.689	11.793	1.00 19.61	7
		663 CA THR	82	9.642	64.463	11.680	1.00 18.45	6
	ATOM	664 CB THR	82	9.316	62.950	11.683	1.00 25.98	6
2 5	ATOM	665 OG1 THR	82	9.907	62.351	10.527	1.00 18.89	8
35	ATOM	666 CG2 THR	82	7.795	62.775	11.666	1.00 24.98	6
	ATOM	667 C THR	82	8.971	65.100	12.891	1.00 16.02	6
	MOTA	668 O THR	82	9.248	64.735	14.035	1.00 14.79	8
	ATOM	669 N VAL	83	8.075	66.045	12.647	1.00 16.23	7
	ATOM	670 CA VAL	83	7.451	66.758	13.753	1.00 16.97	6
40	ATOM	671 CB VAL	83	7.559	68.282	13.530	1.00 12.81	6
	ATOM	672 CG1 VAL	83	7.051	68.972	14.799	1.00 15.92	6
	ATOM	673 CG2 VAL	83	8.986	68.760	13.246	1.00 13.32	
	ATOM	674 C VAL	83	6.020	66.264			6
	ATOM	675 O VAL	83	5.261		13.892	1.00 19.97	6
45	ATOM				66.329	12.918	1.00 18.57	8
10	ATOM		84	5.686	65.756	15.075	1.00 16.89	7
			84	4.372	65.188	15.312	1.00 19.89	6
	ATOM	678 CB LEU	84	4.621	63.786	15.890	1.00 18.15	6
	ATOM	679 CG LEU	84	5.491	62.863	15.021	1.00 23.40	6
	ATOM	680 CD1 LEU	84	5.927	61.690	15.868	1.00 25.20	6
50	ATOM	681 CD2 LEU	84	4.752	62.396	13.758	1.00 20.46	6
	ATOM	682 C LEU	84		66.016	16.228	1.00 22.29	6
	ATOM	683 O LEU	84		66.891		1.00 23.90	8
	ATOM	684 N PHE	85		65.750	16.218	1.00 23.90	7
	ATOM	685 CA PHE	85		66.444			
55	ATOM	686 CB PHE	85			17.111	1.00 22.92	6
	ATOM				67.431	16.333	1.00 21.76	6
			85		68.350	17.184	1.00 27.90	6
	ATOM	688 CD1 PHE	85		69.013	18.266	1.00 28.30	6
	ATOM	689 CD2 PHE	85		68.533	16.899	1.00 26.61	6
CO	MOTA	690 CE1 PHE	85	-0.664	69.874	19.040	1.00 29.65	6
60	ATOM	691 CE2 PHE	85	-2.559	69.386	17.668	1.00 25.61	6
	ATOM	692 CZ PHE	85		70.047	18.733	1.00 28.75	6
	ATOM	693 C PHE	85		65.399	17.852	1.00 21.99	6
	ATOM	694 O PHE	85		65.000	17.426	1.00 22.11	8
	ATOM	695 N GLU	86		64.883		1.00 22.11	
65	ATOM	696 CA GLU	86			18.938		7
-	ATOM				63.762	19.702	1.00 18.04	6
	ATOM		86 86		52.463	19.210	1.00 20.84	6
			86		51.815	17.911	1.00 25.05	6
	ATOM	699 CD GLU	86		51.048	17.019	1.00 41.96	6
70	ATOM	700 OE1 GLU	86		50.507	17.416	1.00 46.14	8
70	ATOM	701 OE2 GLU	86		0.893	15.765	1.00 40.77	8
	ATOM	702 C GLU	86	0.694	4.026	21.176	1.00 18.46	6

	ATOM ATOM ATOM	703 704 705	N 7	ELU 86 RP 87	0.031		21.462 22.156 23.553	1.00 12.60	8 7 6
5	ATOM ATOM	706 707	CB T	RP 87	-0.808	63.056 64.023	24.411 24.687	1.00 18.40	6
	MOTA	708		RP 87			25.521		6
	ATOM ATOM	709 710	CE2 T	'RP 87 'RP 87		65.805 65.738	25.526 26.255	1.00 24.31 1.00 24.84	6 6
10	ATOM		CD1 T				24.231		6
10	ATOM ATOM	713		'RP 87 'RP 87		65.069 66.966	24.734 26.266		7 6
	ATOM		CZ3 T			66.890 67.499	26.987	1.00 29.83	6
	ATOM ATOM		CH2 T	RP 87		62.967	26.970 24 .068	1.00 29.09 1.00 15.44	6 6
15	ATOM ATOM			RP 87 EU 88	2.178 2.036	63.499 61.873	25.018 23.447	1.00 16.68 1.00 14.44	8 7
	ATOM	719	CA L	E U 88	3.153	61.051	23.861	1.00 20.07	6
	ATOM ATOM			EU 88	2.596 3.608	59.942 59.303	24.783 25.769	1.00 17.49 1.00 16.97	6 6
20	MOTA	722	CD1 L	EU 88	4.062	60.299	26.830	1.00 17.38	6
	ATOM ATOM		CD2 L	EU 88	2.987 3.889	58.053 60.399	26.370 22.677	1.00 13.93 1.00 20.44	6 6
	ATOM	725	O L	EU 88	3.255	59.857	21.752	1.00 19.65	8
25	ATOM ATOM			AL 89 AL 89	5.218 5.998	60.517 59.926	22.620 21.542	1.00 18.11 1.00 14.66	7 6
	ATOM	728	CBA V	AL 89	6.686	61.029	20.699	0.50 7.52	6
	ATOM ATOM		CBB V CG1 V		6.677 7.573	60.941 61.890	20.604 21.597	0.50 13.86 0.50 7.13	6 6
20	ATOM	731	CG1 V	AL 89	5.696	61.409	19.543	0.50 15.87	6
30	ATOM ATOM		CG2 V. CG2 V.		7.501 7.264	60.486 62.090	19.531 21.402	0.50 3.91 0.50 18.65	6 6
	MOTA	734	C V	AL 89	7.109	59.032	22.107	1.00 15.71	6
	ATOM ATOM			AL 89 EU 90	7.6 8 9 7.379	59.262 57.958	23.179 21.386	1.00 14.52 1.00 15.13	8 7
35	MOTA	737	CA L	EU 90	8.520	57.133	21.703	1.00 13.72	6
	ATOM ATOM			EU 90 EU 90	8.287 9.650	55.625 54.978	21.488 21.873	1.00 17.87 1.00 26.07	6 6
	ATOM	740	CD1 L	eu 90	9.479	54.066	23.036	1.00 30.57	6
40	MOTA MOTA		CD2 L	EU 90 EU 90	10.373 9.657	54.463 57.674	20.662 20.803	1.00 25.07 1.00 17.58	6 6
	ATOM	743	o L	EU 90	9.611	57.517	19.576	1.00 14.46	8
	ATOM ATOM			LN 91 LN 91	10.673 11.745	58.298 58.908	21.412 20.623	1.00 15.83 1.00 17.70	7 6
A E	ATOM	746	CB G	LN 91	12.252	60.238	21.264	1.00 15.03	6
45	atom atom			LN 91 LN 91	11.105 11.564	61.231 62.636	21.472 21.868	1.00 12.81 1.00 15.79	6 6
	MOTA	749 (DE1 G	LN 91	12.023	62.823	22.988	1.00 14.61	8
	atom atom		NE2 GI	LN 91 LN 91	11.409 12. 9 71	63.610 58.042	20.984	1.00 16.27 1.00 17.71	7 6
50	MOTA	752 () G1	LN 91	13.370	57.296	21.268	1.00 19.37	8
	ATOM ATOM			IR 92 IR 92	13.607 14.853	58.207 57.488	19.218 18.934	1.00 14.05 1.00 19.01	7 6
	ATOM		CB TF	IR 92	14.562	56.225	18.089	1.00 16.40	6
55	ATOM ATOM		G1 TE		15.769 13.943	55.485 56.499	17.905 16.720	1.00 18.39 1.00 10.45	8 6
	MOTA	758 C	TH.	IR 92	15.803	58.416	18.173	1.00 18.96	6
	ATOM ATOM	759 C			15.339 17.095	59.272 58.153	17.409 18.251	1.00 21.88 1.00 18.78	8 7
60	ATOM	761 C	D PF	0 93	17.747	57.169	19.135	1.00 22.16	6
00	ATOM ATOM		:A PF :B PF		18.090 19.352	58.929 58.803	17.530 18.371	1.00 24.37 1.00 24.99	6 6
	ATOM	764 C	G PF	0 93	19.162	57.609	19.235	1.00 26.05	6
	ATOM ATOM	765 C			18.285 18.852	58.362 59.019	16.138 15.248	1.00 27.02 1.00 27.04	6 8
65	MOTA	767 N	HI	s 94	17.978	57.069	15.960	1.00 24.22	7
	MOTA MOTA		A HI B HI		18.114 19.444	56.421 55.690	14.651 14.439	1.00 25.72 1.00 20.09	6 6
	MOTA	770 C	G HI	s 94	20.639	56.587	14.595	1.00 21.67	6
70	ATOM ATOM		D2 HI D1 HI		21.161 21.380	57.530 56.595	13.798 15.754	1.00 23.30 1.00 27.49	6 7
. •	ATOM		E1 HI		22.338	57.501	15.657	1.00 26.54	6

	ATOM	774	NE2	HIS	94	22.211	58.078	14.482	1.00 32.10	7
	ATOM	775	C	HIS	94	17.038	55.350	14.453	1.00 24.49	6
	MOTA	776	0	HIS	94	16.481	54.838	15.429	1.00 24.01	8
_	ATOM	7 77	N	LEU	95	16.847	54.929	13.214	1.00 21.96	7
5	MOTA	778	CA	LEU	95	15.900	53.847	12.960	1.00 26.06	6
	ATOM	779	CB	LEU	95	15.014	54.118	11.741	1.00 26.66	6
	ATOM	780	CG CD1	LEU LEU	95 95	13.994 13.449	55.248 55.601	11.899 10.525	1.00 35.19 1.00 25.66	6 6
	MOTA MOTA	781 782	CD2		95 95	12.895	54.908	12.900	1.00 24.13	6
10	ATOM	783	C	LEU	95	16.626	52.525	12.720	1.00 26.30	6
10	ATOM	784	ŏ	LEU	95	15.999	51.464	12.790	1.00 26.83	8
	MOTA	785	N	GLU	96	17.884	52.601	12.326	1.00 25.44	7
	ATOM	786	CA	GLU	96	18.688	51.413	12.087	1.00 28.55	6
- ·	ATOM	787	CB	GLU	96	19.062	51.144	10.634	1.00 28.97	6
15	MOTA	788	CG	GLU	96	17.977	51.334	9.605	1.00 34.46	6
	MOTA	789	CD	GLU	96 06	18.414	51.109	8.168	1.00 42.07 1.00 41.53	6 8
	MOTA	790 791	OE1	GLU GLU	96 96	19.560 17.592	50.709 51.343	7.882 7.256	1.00 41.33	8
	MOTA MOTA	792	C	GLU	96	19.995	51.575	12.885	1.00 32.22	6
20	ATOM	793	Ö	GLU	96	20.525	52.686	13.015	1.00 31.68	8
20	ATOM	794	N	PHE	97	20.396	50.487	13.538	1.00 29.38	7
	ATOM	795	CA	PHE	97	21.622	50.447	14.315	1.00 31.45	6
	ATOM	796	CB	PHE	97	21.388	50.351	15.832	1.00 29.88	6
	MOTA	797	CG	PHE	97	20.640	51.497	16.464	1.00 28.91	6
25	ATOM	798		PHE	97	19.256	51.580	16.386	1.00 19.88	6
	MOTA	799		PHE	97	21.311	52.503	17.131	1.00 27.06	6 6
	ATOM ATOM	800 801		PHE PHE	97 97	18.557 20.622	52.624 53.545	16.971 17.719	1.00 23.29 1.00 23.27	6
	ATOM	802	CZ	PHE	97	19.244	53.626	17.636	1.00 25.87	6
30	ATOM	803	c	PHE	97	22.455	49.233	13.861	1.00 31.11	6
	ATOM	804	ō	PHE	97	22.007	48.334	13.164	1.00 32.31	8
	ATOM	805	N	GLN	98	23.726	49.213	14.219	1.00 34.14	7
	ATOM	806	CA	GLN	98	24.636	48.131	13.939	1.00 33.31	6
2.5	MOTA	807	CB	GLN	98	26.042	48.629	13.635	1.00 38.15	6
35	MOTA	808	CG	GLN	98	26.207	49.422	12.356	1.00 45.65 1.00 49.99	6 6
	ATOM ATOM	809 810	CD OF1	GLN GLN	98 98	25.763 26.455	48.712 47.828	11.097 10.589	1.00 52.58	8
	ATOM	811	NE2	GLN	98	24.603	49.088	10.563	1.00 53.06	7
	ATOM	812	C	GLN	98	24.662	47.218	15.172	1.00 31.48	6
40	ATOM	813	Ō	GLN	98	24.459	47.664	16.300	1.00 27.98	8
	MOTA	814	N	GLU	99	24.990	45.955	14.920	1.00 30.75	7
	ATOM	815	CA	GLU	99	25.112	44.978	16.009	1.00 32.56	6
	MOTA	816	CB	GLU	99	25.598	43.653	15.420	1.00 36.89	6
45	MOTA	817	CG	GLU	99	25.204	42.392	16.141	1.00 44.86 1.00 48.45	6 6
40	MOTA MOTA	818 819	CD OE1	GLU	99 99	24.771 23.802	41.288 40.573	15.184 15.521	1.00 53.90	8
	ATOM	820	OE2	GLU	99	25.400	41.148	14.118	1.00 50.56	8
	MOTA	821	C	GLU	99	26.130	45.551	16.980	1.00 31.14	6
	ATOM	822	ō	GLU	99	27.136	46.048	16.475	1.00 31.94	8
50	ATOM	823	N	GLY	100	25.919	45.571	18.275	1.00 32.19	7
	MOTA	824	CA	GLY	100	26.874	46.123	19.217	1.00 31.10	6
	ATOM	825	C	GLY	100	26.643	47.541	19.696	1.00 31.51	6
	ATOM	826	0	GLY	100	27.082	47.931	20.789	1.00 30.30	8
55	ATOM	827 828	N CA	GLU GLU	101 101	25.948 25.675	48.369 49.746	18.921 19.297	1.00 34.41 1.00 34.07	7 6
55	ATOM ATOM	829	CB	GLU	101	24.949	50.452	18.148	1.00 37.86	6
	ATOM	830	CG	GLU	101	25.777	50.676	16.889	1.00 48.38	6
	ATOM	831	CD	GLU	101	24.984	51.520	15.895	1.00 49.17	6
	ATOM	832	OE1	GLU	101	24.251	52.408	16.385	1.00 58.51	8
60	ATOM	833	OE2	GLU	101	25.046	51.333	14.669	1.00 48.56	8
	ATOM	834	С	GLU	101	24.783	49.848	20.537	1.00 33.06	6
	ATOM	835	0	GLU	101	24.086	48.888	20.886	1.00 27.70	8
	ATOM	836	N	THR	102	24.747	51.057	21.107	1.00 31.92	7
65	ATOM ATOM	837 838	CA CB	THR THR	102 102	23.870 24.508	51.303 52.161	22.248 23.341	1.00 32.85 1.00 35.75	6 6
00	ATOM	839	OG1	THR	102	25.546	51.438	24.021	1.00 35.75	8
	ATOM	840	CG2	THR	102	23.532	52.577	24.441	1.00 35.82	6
	ATOM	841	c	THR	102	22.582	51.944	21.721	1.00 32.54	6
	MOTA	842	0	THR	102	22.650	52.932	20.991	1.00 30.03	8
70	MOTA	843	N	ILE	103	21.431	51.329	22.014	1.00 28.53	7
	MOTA	844	CA	ILE	103	20.162	51.939	21.590	1.00 25.40	6

	ATOM	845	CB	ILE	103	19.131	50.873	21.163	1.00 26.58	6
	ATOM	846	CG2	ILE	103	17.776	51.496	20.828	1.00 25.47	6
	ATOM	847	CG1	ILE	103	19.669	50.080	19.971	1.00 21.79	6
	MOTA	848	CD1	ILE	103	18.739	49.003	19.438	1.00 19.73	6
5	MOTA	849	С	ILE	103	19.624	52.753	22.767	1.00 25.27	6 8
	ATOM	850	0	ILE	103	19.439	52.181	23.853 22.591	1.00 23.06 1.00 24.90	7
	MOTA	851	N	MET	104	19.443	54.059		1.00 24.30	6
	ATOM	852	CA	MET	104	18.893 19.797	54.913 56.097	23.639 23.963	1.00 21.33	6
1.0	MOTA	853	CB	MET	104	20.810	55.826	25.101	1.00 29.68	6
10	ATOM	854	CG	MET	104 104	21.940	57.256	25.242	1.00 46.02	16
	MOTA	855 856	SD CE	MET MET	104	22.667	57.216	23.589	1.00 31.10	6
	MOTA MOTA	856 857	C	MET	104	17.528	55.456	23.215	1.00 21.27	6
	ATOM	858	Ö	MET	104	17.374	55.991	22.106	1.00 22.96	8
15	ATOM	859	N	LEU	105	16.503	55.242	24.027	1.00 20.55	7
10	ATOM	860	CA	LEU	105	15.134	55.668	23.728	1.00 22.33	6
	ATOM	861	CB	LEU	105	14.192	54.450	23.550	1.00 14.66	6
	MOTA	862	CG	LEU	105	14.713	53.389	22.561	1.00 18.89	6
	ATOM	863	CD1	LEU	105	13.796	52.178	22.489	1.00 19.44	6
20	MOTA	864		LEU	105	14.882	54.056	21.186	1.00 18.70	6
	MOTA	865	С	LEU	105	14.567	56.559	24.817	1.00 20.15	6 8
	ATOM	866	0	LEU	105	15.050	56.506	25.950	1.00 18.39	7
	MOTA	867	N	ARG	106	13.523	57.324	24.483	1.00 18.25	6
0.5	MOTA	868	CA	ARG	106	12.912	58.174	25.516 25.508	1.00 17.07	6
25	MOTA	869	CB	ARG	106	13.607 12.834	59.553 60.597	26.290	1.00 14.30	6
	ATOM	870	CG	ARG	106 106	13.699	61.788	26.757	1.00 19.51	6
	MOTA	871 872	CD NE	ARG ARG	106	13.334	62.927	26.025	1.00 23.46	7
	ATOM ATOM	873	CZ	ARG	106	12.990	64.174	26.065	1.00 24.43	6
30	ATOM	874		ARG	106	12.923	64.892	27.176	1.00 25.93	7
J 0	ATOM	875		ARG	106	12.697	64.795	24.936	1.00 18.72	7
	ATOM	876	С	ARG	106	11.422	58.321	25.304	1.00 18.56	6
	ATOM	877	0	ARG	106	10.998	58.479	24.142	1.00 20.43	8
	ATOM	878	N	CYS	107	10.642	58.246	26.378	1.00 15.23	7
35	MOTA	879	CA	CYS	107	9.189	58.419	26.292	1.00 14.89	6 6
	ATOM	880	C	CYS	107	8.934	59.891	26.583	1.00 15.28 1.00 15.96	8
	ATOM	881	0	CYS	107	9.296 8.438	60.294 57.565	27.690 27.322	1.00 14.55	6
	ATOM	882 883	CB SG	CYS CYS	107 107	6.691	57.368	27.013	1.00 13.91	16
40	MOTA ATOM	884	N	HIS	108	8.446	60.653	25.604	1.00 15.07	7
40	ATOM	885	CA	HIS	108	8.334	62.103	25.811	1.00 11.91	6
	ATOM	886	CB	HIS	108	9.190	62.757	24.708	1.00 16.03	6
	ATOM	887	CG	HIS	108	9.119	64.240	24.572	1.00 16.94	6
	ATOM	888	CD2	HIS	108	9.068	65.023	23.462	1.00 17.64	6
45	ATOM	889	ND1	HIS	108	9.103	65.108	25.657	1.00 17.41	7
	ATOM	890		HIS	108	9.034	66.350	25.215	1.00 17.37	6
	ATOM	891		HIS	108	9.021	66.333	23.895	1.00 20.00	7 6
	ATOM	892	C	HIS	108	6.925	62.647	25.733 24.762	1.00 12.54	8
F 0	ATOM	893	0	HIS	108	6.224	62.361	26.654	1.00 12.34	7
50	ATOM	894	N	SER	109	6.515 5.160	63.502 64.091	26.605	1.00 11.70	6
	ATOM	895 896	CA	SER	109 109	4.583	64.134		1.00 13.47	ő
	ATOM		CB OG	SER	109	5.609	64.845	28.800	1.00 16.16	8
	ATOM	897 898	C	SER SER	109	5.190	65.459	25.970	1.00 14.21	6
55	ATOM ATOM	899	Ö	SER	109	6.180	66.232	25.903	1.00 14.63	8
<i>33</i>	ATOM	900	N	TRP	110	4.047	65.804	25.381	1.00 16.58	7
	ATOM	901	CA	TRP	110	3.860	67.102	24.708	1.00 16.04	6
	ATOM	902	CB	TRP	110	2.480	67.158	24.072	1.00 18.73	6
	ATOM	903	CG	TRP	110	2.187	68.425	23.306	1.00 21.24	6
60	ATOM	904		TRP	110	1.135	69.339	23.589	1.00 20.70	6
	ATOM	905		TRP	110	1.193	70.361	22.616	1.00 25.92	6
	ATOM	906	CE3	TRP	110	0.112	69.372	24.549	1.00 24.16	6
	ATOM	907	CD1	TRP	110	2.827	68.908	22.214	1.00 22.22	6
	ATOM	908		TRP	110	2.233	70.069	21.765	1.00 22.81	7
65	ATOM	909		TRP	110	0.276	71.404	22.568	1.00 24.18	6
	ATOM	910		TRP	110	-0.781	70.434	24.509	1.00 30.15	6
	ATOM	911		TRP	110	-0.698	71.433	23.526	1.00 31.04	6 6
	ATOM	912	С	TRP	110	4.082	68.245	25.681	1.00 14.44 1.00 17.08	8
70	MOTA	913	0	TRP	110 111	3.665 4.928	68.219 69.199	26.852 25.294	1.00 17.08	7
70	MOTA	914 915	N CA	LYS LYS	111	5.347	70.325	26.115	1.00 19.40	6
	ATOM	713	~~	44.5						

	ATOM	916	CB	LYS	111	4.131	71.241	26.418	1.00 21.00	6
	ATOM	917	CG	LYS	111	3.583	71.904	25.155	1.00 24.94	6 6
	MOTA	918 919	CD CE	LYS LYS	111 111	2.124 1.952	72.287 73.719	25.337 25.781	1.00 34.17	6
5	ATOM ATOM	920	NZ	LYS	111	2.783	74.668	24.987	1.00 52.66	7
Ŭ	ATOM	921	C	LYS	111	5.940	69.921	27.450	1.00 20.33	6
	ATOM	922	0	LYS	111	5.905	70.694	28.419	1.00 16.80	8
	ATOM	923	N	ASP	112	6.444	68.695	27.602	1.00 18.28	7
1.0	ATOM	924	CA	ASP	112	6.989	68.233	28.861	1.00 20.31 1.00 24.52	6 6
10	ATOM ATOM	925 926	CB CG	ASP ASP	112 112	8.242 9.306	69.088 68.737	29.191 28.155	1.00 24.32	6
	ATOM	927	OD1		112	9.700	67.545	28.119	1.00 39.68	8
	ATOM	928	OD2		112	9.719	69.588	27.360	1.00 35.00	8
	ATOM	929	С	ASP	112	6.015	68.203	30.018	1.00 23.40	6
15	MOTA	930	0	ASP	112	6.426	68.475	31.148	1.00 23.42	8
	ATOM	931	N	LYS	113	4.731	67.889	29.785	1.00 23.10 1.00 22.35	7 6
	ATOM ATOM	932 933	CA CB	LYS LYS	113 113	3.792 2.352	67.721 67.432	30.891 30.437	1.00 22.33	6
	ATOM	934	CG	LYS	113	1.758	68.611	29.659	1.00 27.09	6
20	ATOM	935	CD	LYS	113	0.232	68.574	29.608	1.00 28.34	6
	ATOM	936	CE	LYS	113	-0.269	69.780	28.816	1.00 32.92	6
	MOTA	937	NZ	LYS	113	-0.196	71.075	29.554	1.00 33.55	7
	ATOM	938	C	LYS	113	4.352	66.597	31.748	1.00 19.86 1.00 21.45	6 8
25	ATOM ATOM	939 940	O N	LYS PRO	113 114	4.890 4.288	65.603 66.761	31.264 33.066	1.00 21.43	7
23	ATOM	941	CD	PRO	114	3.701	67.928	33.768	1.00 16.95	6
	ATOM	942	CA	PRO	114	4.923	65.801	33.957	1.00 17.00	6
	MOTA	943	CB	PRO	114	4.548	66.292	35.342	1.00 19.22	6
20	MOTA	944	CG	PRO	114	4.169	67.733	35.176	1.00 21.34	6
30	MOTA	945	C	PRO	114	4.451	64.405	33.636	1.00 16.83	6 8
	MOTA ATOM	946 947	o N	PRO LEU	114 115	3.237 5.414	64.125 63.483	33.512 33.560	1.00 15.95	7
	ATOM	948		LEU	115	5.081	62.104	33.215	1.00 17.10	6
	ATOM	949	CB	LEU	115	5.769	61.879	31.856	1.00 16.83	6
35	MOTA	950		LEU	115	5.790	60.498	31.231	1.00 21.64	6
	ATOM	951	CD1		115	4.399	60.132	30.733	1.00 19.24	6
	ATOM	952	CD2		115	6.77 7	60.486	30.043	1.00 19.80 1.00 21.13	6 6
	MOTA MOTA	953 954	С 0	LEU LEU	115 115	5.606 6.788	61.116 61.200	34.226 34.569	1.00 21.13	8
40	ATOM	955		VAL	116	4.839	60.105	34.630	1.00 20.51	7
	ATOM	956		VAL	116	5.314	59.073	35.545	1.00 20.40	6
	MOTA	957		VAL	116	4.787	59.277	36.971	1.00 18.72	6
	MOTA	958	CG1		116	5.313	60.547	37.644	1.00 22.67	6
45	MOTA	959	CG2	VAL	116 116	3.257 4.807	59.328 57.703	36.998 35.073	1.00 22.12 1.00 19.73	6 6
40	MOTA MOTA	960 961		VAL	116	3.910	57.682	34.223	1.00 20.76	8
	ATOM	962		LYS	117	5.268	56.615	35.693	1.00 17.34	7
	MOTA	963		LYS	117	4.760	55.290	35.381	1.00 20.33	6
	ATOM	964		LYS	117	3.271	55.182	35.802	1.00 21.74	6
50	ATOM	965		LYS	117	3.115	54.927	37.301	1.00 24.43	6
	MOTA MOTA	966		LYS	117	1.793 0.798	55.445	37.832 38.056	1.00 32.69	6 6
	ATOM	967 968		LYS LYS	117 117	-0.568	54.314 54.865	38.266	1.00 40.27	7
	ATOM	969		LYS	117	4.956	54.936	33.914	1.00 18.58	6
55	ATOM	970		LYS	117	4.026	54.535	33.234	1.00 24.35	8
	ATOM	971		VAL	118	6.181	55.063	33.417	1.00 20.45	7
	MOTA	972		VAL	118	6.542	54.798	32.039	1.00 19.15	6
	ATOM	973		VAL	118	7.756 8.199	55.643	31.607 30.176	1.00 12.17 1.00 18.94	6 6
60	ATOM ATOM	974 975	CG1 CG2		118 118	7.408	55.396 57.129	31.794	1.00 16.75	6
00	ATOM	976		VAL	118	6.868	53.330	31.797	1.00 18.58	6
	ATOM	977		VAL	118	7.606	52.717	32.564	1.00 17.16	8
	MOTA	978	N	THR	119	6.307	52.803	30.711	1.00 15.94	7
~ F	MOTA	979		THR	119	6.527	51.425	30.335	1.00 16.50	6
65	MOTA	980		THR	119	5.291	50.523	30.367	1.00 19.59	6
	ATOM	981 982	OG1 CG2		119 119	4.770 5.695	50.410 49.123	31.693 29.872	1.00 23.11 1.00 24.83	8 6
	ATOM ATOM	982		THR	119	7.053	51.424	29.872	1.00 24.83	6
	ATOM	984		THR	119	6.436	52.130	28.095	1.00 14.36	8
70	MOTA	985		PHE	120	8.121	50.679	28.643	1.00 14.86	7
	MOTA	986	CA	PHE	120	8.616	50.608	27.259	1.00 13.85	6

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	MOTA	987	CB PH			50.797	27.240	1.00 15.51	6
	MOTA	988	CG PH			52.230	27.463	1.00 13.38	6
	MOTA	989	CD1 PH			52.701	28.750	1.00 20.15	6
-	MOTA	990	CD2 PH			53.051	26.381	1.00 20.08	6
5	MOTA	991	CE1 PH			54.002	28.953	1.00 17.14	6
	ATOM	992	CE2 PH			54.367	26.578	1.00 22.12	6
	MOTA	993	CZ PH			54.818	27.867	1.00 17.10	6
	ATOM	994	C PH			49.216	26.721	1.00 17.13	6
10	MOTA	995	O PH			48.221	27.407	1.00 14.78	8
10	MOTA	996	N PH			49.166	25.575	1.00 16.20	7
	ATOM	997	CA PH			47.868	25.011	1.00 18.83	6
	MOTA	998	CB PH			47.821	24.616	1.00 13.50	6
	MOTA	999	CG PH			48.052	25.656	1.00 18.60	6
1-	ATOM	1000	CD1 PH			49.339	26.017	1.00 17.37	6
15	MOTA	1001	CD2 PH			46.961	26.334	1.00 18.44	6
	MOTA	1002	CE1 PH			49.524	27.006	1.00 19.78	6
	ATOM	1003	CE2 PH			47.173	27.313	1.00 22.69	6
	MOTA	1004	CZ PH			48.445	27.660	1.00 15.74	6
	MOTA	1005	C PH			47.539	23.749	1.00 18.44	6
20	MOTA	1006	O PH			48.454	22.987	1.00 15.63	8
	ATOM	1007	N GI			46.253	23.480	1.00 19.35	7
	MOTA	1008	CA GI			45.880	22.203	1.00 19.90	6
	MOTA	1009	CB GI			45.379	22.317	1.00 16.32	6
0.5	ATOM	1010	CG GI			44.583	21.065	1.00 18.39	6
25	MOTA	1011	CD GI			43.764	21.247	1.00 21.98	6
	MOTA	1012	OE1 GI			43.461	22.374	1.00 19.18	8
	ATOM	1013	NE2 GL		12.700	43.396	20.153	1.00 24.51	7
	MOTA	1014	C GI			44.774	21.609	1.00 15.34	6
20	MOTA	1015	O GI		7.789	43.832	22.321	1.00 17.30	8
30	MOTA	1016	N AS			44.931	20.439	1.00 18.98	7
	MOTA	1017	CA AS			43.975	19.859	1.00 22.95	6
	MOTA	1018	CB AS			42.708	19.332	1.00 19.57	6
	MOTA	1019	CG AS			43.130	18.244	1.00 26.31	6
2.5	MOTA	1020	OD1 AS			44.053	17.441	1.00 19.76	8 7
35	ATOM	1021	ND2 AS		9.375	42.463	18.213	1.00 28.57 1.00 21.02	6
	ATOM	1022	C AS			43.643	20.803	1.00 21.02	8
	ATOM	1023	O AS			42.525 44.632	21.579	1.00 19.77	7
	ATOM	1024	N GL		4.951 3.852	44.516	22.495	1.00 15.77	6
40	ATOM	1025 1026	CA GL		4.159	43.885	23.844	1.00 14.85	6
40	ATOM ATOM	1027	O GL		3.210	43.658	24.611	1.00 15.05	8
	ATOM	1028	N LY		5.405	43.610	24.133	1.00 13.81	7
	ATOM	1029	CA LY		5.830	42.997	25.379	1.00 21.18	6
	ATOM	1030	CB LY		6.700	41.738	25.247	1.00 14.85	6
45	ATOM	1031	CG LY		6.934	41.032	26.559	1.00 16.28	6
10	ATOM	1032	CD LY		7.406	39.587	26.281	1.00 22.51	6
	ATOM	1033	CE LY		7.925	38.989	27.587	1.00 30.62	6
	ATOM	1034	NZ LY		8.822	37.818	27.330	1.00 36.72	7
	ATOM	1035	C LY		6.725	44.014	26.121	1.00 18.20	6
50	ATOM	1036	O LY		7.648	44.525	25.509	1.00 19.98	8
	ATOM	1037	N SE		6.385	44.216	27.393	1.00 17.62	7
	ATOM	1038	CA SE	R 126	7.107	45.241	28.155	1.00 20.03	6
	ATOM	1039	CB SE		6.355	45.459	29.485	1.00 23.22	6
	ATOM	1040	OG SE		7.317	45.773	30.466	1.00 38.12	8
5 5	ATOM	1041	C SE		8.541	44.823	28.389	1.00 17.85	6
	ATOM	1042	O SE	R 126	8.842	43.657	28.647	1.00 21.31	8
	ATOM	1043	N GL	N 127	9.490	45.718	28.254	1.00 17.16	7
	ATOM	1044	CA GL	N 127	10.898	45.515	28.408	1.00 17.45	6
	ATOM	1045	CB GL	N 127	11.723	46.073	27.225	1.00 20.82	6
60	ATOM	1046	CG GL	N 127	11.352	45.419	25.897	1.00 18.56	6
	ATOM	1047	CD GL	N 127	11.497	43.912	25.927	1.00 24.44	6
	ATOM	1048	OE1 GL	N 127	12.606	43.416	26.116	1.00 31.62	8
	MOTA	1049	NE2 GL	N 127	10.436	43.130	25.773	1.00 19.15	7
	ATOM	1050	C GL		11.386	46.251	29.661	1.00 20.94	6
65	MOTA	1051	O GL		12.439	45.929	30.179	1.00 18.25	8
	MOTA	1052	N LY		10.643	47.285	30.032	1.00 21.18	7
	MOTA	1053	CA LY		11.070	48.048	31.216	1.00 23.10	6
	ATOM	1054	CB LY		12.177	49.034	30.842	1.00 21.83	6
m A	MOTA	1055	CG LY		12.683	49.882	32.013	1.00 24.67	6
70	MOTA	1056	CD LY		13.739	50.905	31.589	1.00 18.23	6
	MOTA	1057	CE LY	s 128	14.048	51.746	32.870	1.00 27.02	6

	ATOM	1058	NZ	LYS	128	15.081	52.794	32.574	1.00 24.24	7
	ATOM	1059		LYS	128	9.884				6
	ATOM	1060		LYS	128	9.193				8
5	ATOM ATOM	1061 1062		PHE PHE	129	9.678	48.822			7
3	ATOM	1062		PHE	129 129	8.708 7.610	49.695 48.926			6 6
	ATOM	1064			129	6.772	49.837			6
	MOTA	1065		1 PHE	129	5.799				6
1.0	ATOM	1066		2 PHE	129	7.002	49.928	36.700	1.00 29.98	6
10	ATOM	1067		1 PHE	129	5.026	51.491			6
	MOTA MOTA	1068 1069		2 PHE PHE	129 129	6.2 49 5.262	50.788	37.491		6
	ATOM	1070		PHE	129	9.480	51.574 50.577	36.902 34.687		6 6
	ATOM	1071		PHE	129	10.388	50.049	35.359		8
15	ATOM	1072	N	SER	130	9.134	51.846	34.853		7
	ATOM	1073		SER	130	9.779	52.641	35.917		6
	MOTA	1074		SER	130	11.025	53.344	35.422		6
	ATOM ATOM	1075 1076		SER SER	130 130	11.271 8.777	54.465	36.250		8
20	ATOM	1077		SER	130	8.123	53.667 54.285	36.434 35.576		6 8
	ATOM	1078		HIS	131	8.668	53.889	37.730		7
	MOTA	1079	CA	HIS	131	7.710	54.901	38.204	1.00 23.65	6
	ATOM	1080		HIS	131	7.604	54.918	39.737	1.00 28.35	6
25	ATOM	1081		HIS	131	6.859	53.706	40.197	1.00 23.57	6
23	ATOM ATOM	1082 1083		HIS	131 131	7.307	52.509	40.642	1.00 18.55	6
	ATOM	1084		HIS	131	5.478 5.095	53.666 52.478	40.170	1.00 26.69 1.00 16.65	7 6
	ATOM	1085		HIS	131	6.173	51.764	40.890	1.00 23.94	7
	MOTA	1086	С	HIS	131	8.108	56.314	37.814	1.00 23.89	6
30	MOTA	1087	0	HIS	131	7.261	57.205	37.712	1.00 26.21	8
	ATOM	1088	N	LEU	132	9.426	56.548	37.689	1.00 21.77	7
	ATOM ATOM	1089 1090	CA CB	LEU	132 132	9.886	57.900	37.480	1.00 20.70	6
	MOTA	1091	CG	LEU	132	10.630 10.022	58.361 58.084	38.760 40.148	1.00 30.28 1.00 26.56	6 6
35	ATOM	1092		LEU	132	11.073	58.316	41.229	1.00 20.30	6
	MOTA	1093	CD2	LEU	132	8.814	58.980	40.435	1.00 24.99	6
	ATOM	1094	С	LEU	132	10.762	58.144	36.279	1.00 22.94	6
	MOTA	1095	0	LEU	132	10.794	59.326	35.900	1.00 22.01	8
40	ATOM ATOM	1096 1097	N CA	ASP ASP	133 133	11.541 12.469	57.181 57.401	35.778 34.679	1.00 21.75	7
	ATOM	1098	CB	ASP	133	13.560	56.327	34.854	1.00 24.62 1.00 29.71	6 6
	ATOM	1099	CG	ASP	133	14.734	56.321	33.915	1.00 32.90	6
	ATOM	1100		ASP	133	14.837	57.254	33.083	1.00 32.91	8
45	ATOM	1101		ASP	133	15.597	55.394	34.000	1.00 36.01	8
40	MOTA MOTA	1102 1103	С 0	ASP ASP	133 133	11.843	57.230	33.296	1.00 25.88	6
	ATOM	1103	N	PRO	134	11.419 11.857	56.136 58.261	32.940 32.460	1.00 24.36 1.00 24.65	8 7
	ATOM	1105	CD	PRO	134	12.347	59.620	32.778	1.00 22.97	6
	ATOM	1106	CA	PRO	134	11.293	58.185	31.112	1.00 24.00	6
50	MOTA	1107	CB	PRO	134	10.889	59.662	30.870	1.00 24.02	6
	ATOM ATOM	1108	CG	PRO	134	11.987	60.433	31.544	1.00 23.04	6
	ATOM	1109 1110	С 0	PRO PRO	134 134	12.256 11.970	57.764 57.930	30.017	1.00 22.11	6
	ATOM	1111	N	THR	135	13.420	57.212	28.824 30.350	1.00 19.00 1.00 21.43	8 7
55	ATOM	1112	CA	THR	135	14.424	56.805	29.401	1.00 24.98	6
	ATOM	1113	CB	THR	135	15.748	57.584	29.593	1.00 27.24	6
	ATOM	1114		THR	135	16.331	57.065	30.796	1.00 24.99	8
	ATOM	1115		THR	135	15.461	59.069	29.706	1.00 26.07	6
60	MOTA MOTA	1116 1117	С О	THR THR	135 135	14.747	55.312	29.451	1.00 23.58	6
00	ATOM	1118	N	PHE	136	14.445 15.267	54.629 54.790	30.423 28.347	1.00 26.14 1.00 20.63	8 7
	ATOM	1119	CA	PHE	136	15.549	53.391	28.150	1.00 20.03	6
	ATOM	1120	СВ	PHE	136	14.343	52.706	27.523	1.00 25.47	6
C.E.	MOTA	1121	CG	PHE	136	14.408	51.250	27.170	1.00 25.61	6
65	ATOM	1122	CD1		136	14.528	50.270	28.121	1.00 27.00	6
	ATOM ATOM	1123 1124	CD2		136	14.332	50.847	25.841	1.00 27.45	6
	ATOM	1124	CE1		136 136	14.571 14.385	48.929 49.516	27.787 25.490	1.00 32.62 1.00 28.46	6 6
	ATOM	1126	CZ	PHE	136	14.493	48.549	26.463	1.00 20.40	6
70	ATOM	1127	С	PHE	136	16.796	53.197	27.297	1.00 24.00	6
	MOTA	1128	0	PHE	136	16.952	53.801	26.230	1.00 24.50	8

5	MOTA MOTA MOTA MOTA MOTA	1129 1130 1131 1132 1133	CA SER CB SER CG SER C SER	137 137 137 137	17.665 18.914 20.120 20.769 19.128	52.010 52.418 53.559 50.507	27.050 27.908 27.412 26.840	1.00 26.52 1.00 30.03 1.00 44.19 1.00 27.38	7 6 6 8 6	
10	MOTA MOTA MOTA MOTA MOTA	1134 1135 1136 1137 1138	N ILE CA ILE CB ILE	138 138 138	18.911 19.654 20.004 19.189 19.669	49.694 50.164 48.806 48.176 46.748	25.686 25.343 24.193	1.00 25.86 1.00 29.46 1.00 33.38	8 7 6 6	
	MOTA MOTA MOTA	1139 1140 1141 1142	CG1 ILE CD1 ILE C ILE O ILE	138 138 138 138	17.679 16.817 21.477 21.768	48.197 48.155 48.875 49.377	24.472 23.223 24.926 23.849	1.00 30.55 1.00 29.53 1.00 29.88 1.00 27.99	6 6 8	
15	MOTA MOTA MOTA MOTA MOTA	1143 1144 1145 1146 1147	CD PRO CA PRO CB PRO		22.345 22.018 23.776 24.380 23.248	48.476 47.938 48.398 48.213 48.384	25.837 27.184 25.598 26.983 27.950	1.00 31.71 1.00 32.73 1.00 33.85 1.00 36.13 1.00 34.99	7 6 6 6	
20	ATOM ATOM ATOM ATOM	1148 1149 1150 1151	C PRO O PRO N GLN CA GLN	139 139 140 140	24.030 23.324 24.974 25.288	47.160 46.160 47.208 46.110	24.741 24.888 23.827 22.935	1.00 35.63 1.00 38.22 1.00 36.97 1.00 35.17	6 8 7 6	
25	MOTA MOTA MOTA MOTA MOTA	1152 1153 1154 1155 1156	CG GLN CD GLN OE1 GLN	140 140 140 140 140	26.223 27.518 27.883 28.145 27.883	45.124 45.802 45.282 44.084 46.161	23.631 24.088 25.468 25.593 26.468	1.00 43.87 1.00 49.77 1.00 56.21 1.00 57.44 1.00 57.25	6 6 8 7	
30	ATOM ATOM ATOM ATOM ATOM	1157 1158 1159 1160 1161	C GLN O GLN N ALA CA ALA CB ALA	140 140 141 141 141	24.060 23.677 23.473 22.287 21.778	45.418 44.284 46.111 45.634 46.745	22.362 22.693 21.391 20.694 19.774	1.00 34.61 1.00 33.34 1.00 29.80 1.00 30.02 1.00 27.89	6 8 7 6 6	
35	MOTA MOTA MOTA MOTA	1162 1163 1164 1165	C ALA O ALA N ASN CA ASN	141 141 142 142	22.561 23.650 21.528 21.642	44.400 44.270 43.582 42.435	19.832 19.263 19.665 18.738	1.00 29.52 1.00 29.60 1.00 30.60 1.00 31.55	6 8 7 6	
40	ATOM ATOM ATOM ATOM ATOM	1166 1167 1168 1169 1170	CB ASN CG ASN OD1 ASN ND2 ASN C ASN	142 142 142 142 142	21.985 21.012 19.838 21.479 20.357	41.139 40.749 40.423 40.739 42.321	19.453 20.534 20.268 21.781 17.936	1.00 30.39 1.00 31.63 1.00 27.57 1.00 33.23 1.00 32.33	6 8 7 6	
45	ATOM ATOM ATOM ATOM MOTA	1171 1172 1173 1174 1175	O ASN N HIS CA HIS CB HIS CG HIS	142 143 143 143 143	19.453 20.223 19.075 19.262 20.360	43.168 41.257 41.086 39.895 40.234	18.122 17.134 16.266 15.272 14.295	1.00 29.09 1.00 29.40 1.00 28.82 1.00 24.51 1.00 31.72	8 7 6 6 6	
50	ATOM ATOM ATOM ATOM ATOM	1176 1177 1178 1179 1180	CD2 HIS ND1 HIS CE1 HIS NE2 HIS C HIS	143 143 143 143 143	20.704 21.278 22.117 21.794 17.747	41.420 39.328 39.927 41.202 40.857	13.740 13.822 13.008 12.941 16.976	1.00 33.88 1.00 32.86 1.00 31.84 1.00 31.48 1.00 26.62	6 7 6 7 6	
55	ATOM ATOM ATOM ATOM ATOM ATOM	1181 1182 1183 1184 1185 1186	O HIS N SER CA SER CB SER OG SER C SER	143 144 144 144 144	16.696 17.812 16.557 16.839 17.739 15.976	41.098 40.412 40.128 38.979 39.389 41.423	16.366 18.221 18.941 19.915 20.930 19.474	1.00 25.96 1.00 20.85 1.00 24.82 1.00 30.28 1.00 39.11 1.00 24.89	8 7 6 6 8 6	
60	ATOM ATOM ATOM ATOM ATOM	1187 1188 1189 1190 1191	O SER N HIS CA HIS CB HIS CG HIS	144 145 145 145 145	14.775 16.746 16.306 17.474 18.145	41.518 42.522 43.861 44.762 44.212	19.755 19.463 19.811 20.302 21.534	1.00 25.22 1.00 20.33 1.00 19.38 1.00 19.40 1.00 18.37	8 7 6 6	
65	MOTA MOTA ATOM MOTA MOTA	1192 1193 1194 1195 1196	CD2 HIS ND1 HIS CE1 HIS NE2 HIS C HIS	145 145 145 145 145	17.620 19.493 19.768 18.643	43.886 43.965 43.492 43.412 44.553	22.744 21.627 22.829 23.525 18.657	1.00 18.22 1.00 23.55 1.00 26.33 1.00 21.05 1.00 22.05	6 7 6 7 6	
70	ATOM ATOM ATOM	1197 1198 1199	O HIS N SER CA SER	145 146 146	15.013 15.569	45.636 43.997 44.649	18.848 17.440 16.363	1.00 21.86 1.00 20.66 1.00 19.96	8 7 6	

	MOTA MOTA MOTA	1200 1200 1200	l og	SER SER SER	146 146 146	15.075 16.442 13.339	44.15	14.613	1.00 25.61	8
5	MOTA MOTA MOTA	1203 1204 1205	N CA	SER GLY GLY	146 147 147	12.915 12.556 11.123	43.614 45.578 45.383	17.287 16.197	1.00 22.06 1.00 16.70	
10	MOTA MOTA MOTA MOTA	1206 1207 1208 1208	O	GLY GLY ASP ASP	147 147 148	10.385 10.982 9.111	47.762	16.332 16.951	1.00 16.09 1.00 20.62	6 8 7
10	ATOM ATOM ATOM	1210 1211 1212	CB CG	ASP ASP ASP	148 148 148 148	8.324 6.882 6.819 7.849	47.579 47.144	16.674 15.219	1.00 28.99 1.00 41.07	6 6 8
15	ATOM ATOM ATOM	1213 1214 1215	с 0	ASP ASP	148 148 148	5.763 8.315 7.817	46.620 48.214 47.469	14.808 18.590	1.00 39.40 1.00 20.72	8 6 8
20	ATOM ATOM ATOM ATOM	1216 1217 1218 1219	CA CB	TYR TYR TYR TYR	149 149 149 149	8.822 8.811 10.193 11.272	49.966 50.587	20.164 20.472	1.00 18.60 1.00 16.94	7 6 6
	MOTA MOTA MOTA	1220 1221 1222	CD1 CE1 CD2	TYR TYR TYR	149 149 149	11.272 11.901 12.877 11.672	48.928	20.606 19.528 19.737 21.879	1.00 18.45 1.00 19.27 1.00 20.18 1.00 18.36	6 6 6
25	MOTA MOTA MOTA MOTA	1223 1224 1225 1226	CZ OH	TYR TYR TYR	149 149 149	12.636 13.238 14.211	48.216 47.606 46.660	22.116 21.027 21.253	1.00 15.60 1.00 18.77 1.00 18.41	6 6 8
30	MOTA MOTA MOTA	1227 1228 1229	C N CA	TYR TYR HIS HIS	149 149 150 150	7.767 7.539 7.196 6.247	51.061 51.859 51.126 52.171	20.355 19.450 21.559 21.925	1.00 15.78 1.00 15.86 1.00 15.01 1.00 12.99	6 8 7 6
	ATOM ATOM ATOM	1230 1231 1232		HIS HIS	150 150 150	4.849 3.942 2.944	51.980 51.032 51.295	21.372 22.117 23.004	1.00 11.96 1.00 17.71 1.00 16.09	6 6 6
35	ATOM MOTA ATOM ATOM	1233 1234 1235 1236	CE1 NE2 C	HIS HIS HIS	150 150 150 150	3.988 3.058 2.407 6.263	49.660 49.103 50.057 52.270	21.971 22.716 23.370 23.462	1.00 11.60 1.00 16.95 1.00 19.22 1.00 13.37	7 6 7 6
40	ATOM ATOM ATOM ATOM	1237 1238 1239 1240	O N CA C	HIS CYS CYS CYS	150 151 151 151	6.922 5.680 5.670 4.301	51.448 53.355 53.559 53.982	24.129 23.957 25.414 25.880	1.00 12.78 1.00 14.21 1.00 15.38 1.00 16.27	8 7 6 6
45	MOTA MOTA	1241 1242 1243	O CB SG	CYS CYS	151 151 151	3.422 6.746 6.581	54.404 54.562 56.269	25.132 25.856 25.248	1.00 15.15 1.00 16.85 1.00 14.82	8 6 16
40	ATOM ATOM ATOM ATOM	1244 1245 1246 1247	N CA CB OG1	THR THR THR THR	152 152 152 152	4.080 2.875 1.899 2.527	53.805 54.223 53.131 52.212	27.186 27.862 28.305 29.205	1.00 17.41 1.00 17.27 1.00 21.80	7 6 6
50	ATOM ATOM ATOM	1248 1249 1250	CG2 C O	THR THR THR	152 152 152	1.356 3.346 4.471	52.212 52.388 54.989 54.724	27.075 29.127 29.600	1.00 17.53 1.00 17.12 1.00 19.83 1.00 16.21	8 6 6 8
55	ATOM ATOM ATOM ATOM	1251 1252 1253 1254	N CA C O	GLY GLY GLY	153 153 153 153	2.496 2.815 1.647 0.779	55.913 56.706 57.605 57.915	30.731 31.108	1.00 17.84 1.00 20.33 1.00 18.60	7 6 6
	ATOM ATOM ATOM	1255 1256 1257	N CA CB	ASN ASN ASN	154 154 154	1.603 0.560 0.512	58.000 58.815 58.556	30.293 32.373 32.959 34.478	1.00 19.87 1.00 20.99 1.00 20.36 1.00 26.77	8 7 6 6
60	ATOM ATOM ATOM ATOM	1258 1259 1260 1261	OD1 ND2		154 154 154	-0.800 -1.700 -0.927	57.928 58.580 56.639	34.897 35.441 34.633	1.00 40.91 1.00 46.67 1.00 40.24	6 8 7
65	MOTA MOTA MOTA MOTA	1261 1262 1263 1264 1265	O N CA	ASN ILE ILE ILE	154 154 155 155 155	0.879 1.973 -0.018 0.198 0.210	60.300 60.685 61.067 62.514 63.116	32.817 33.272 32.202 32.139 30.731	1.00 22.51 1.00 22.15 1.00 19.40 1.00 22.27 1.00 26.29	6 8 7 6 6
70	ATOM ATOM ATOM ATOM ATOM	1266 1267 1268 1269 1270		ILE	155 155 155 155	0.327 1.367 1.371 -0.974	64.640 62.544 62.874 63.089	30.831 29.899 28.434 32.941	1.00 23.31 1.00 28.16 1.00 29.42 1.00 27.67	6 6 6
	VAI	/ 0	•	- 44 63	155	-2.112	62.726	32.639	1.00 24.10	8

	ATOM ATOM	1271 1272	CA	GLY GLY	156 156	-0.732 -1.942	63.838 64.285	34.780	1.00 37.62	7 6
	ATOM ATOM	1273 1274		GLY GLY	156 156	-2.447 -1.659	63.053 62.512	35.527 36.299		6 8
5	MOTA	1275		TYR	157	-3.655	62.573	35.307		7
	ATOM	1276		TYR	157	-4.182	61.357	35.894	1.00 43.65	6
	ATOM ATOM	1277 1278	CB CG	TYR TYR	157 157	-5.381 -5.020	61.642 62.592	36.832 37.961	1.00 51.51 1.00 57.42	6 6
	ATOM	1279	CD:	1 TYR	157	-5.523	63.885	37.982	1.00 60.45	6
10	ATOM	1280		LTYR	157	-5.179	64.765	38.992	1.00 62.57	6
	MOTA MOTA	1281 1282		TYR TYR	157 157	-4.140 -3.788	62.204 63.079	38.963 39.982	1.00 61.00 1.00 63.03	6 6
	MOTA	1283	CZ	TYR	157	-4.313	64.353	39.986	1.00 63.56	6
1 5	ATOM	1284	OH	TYR	157	-3.979	65.237	40.984	1.00 66.68	8
15	MOTA MOTA	1285 1286	0	TYR TYR	157 157	-4.676 -5.445	60.351 59.420	34.849 35.115	1.00 41.96 1.00 41.33	6 8
	ATOM	1287	N	THR	158	-4.298	60.547	33.594	1.00 36.77	7
	ATOM	1288	CA	THR	158	-4.722	59.693	32.496	1.00 30.71	6
20	ATOM ATOM	1289 1290	CB OG1	THR THR	158 158	-5.260 -6.237	60.597 61.471	31.364	1.00 30.82 1.00 30.47	6
2.0	ATOM	1291		THR	158	-5.851	59.819	31.942 30.207	1.00 30.47	8 6
	MOTA	1292	C	THR	158	-3.532	58.944	31.912	1.00 25.66	6
	ATOM ATOM	1293 1294	0	THR	158	-2.521	59.609	31.642	1.00 24.50	8
25	ATOM	1295	N CA	LEU LEU	159 159	-3.689 -2.617	57.664 56.924	31.609 30.960	1.00 21.00 1.00 21.01	7 6
	ATOM	1296	CB	LEU	159	-2.737	55.435	31.284	1.00 26.53	6
	ATOM	1297	CG	LEU	159	-1.601	54.487	30.958	1.00 27.15	6
	MOTA MOTA	1298 1299		LEU	159 159	-0.323 -1.979	54.817 53.036	31.713 31.316	1.00 25.15 1.00 28.75	6 6
30	ATOM	1300	c	LEU	159	-2.654	57.179	29.461	1.00 22.04	6
	ATOM	1301	0	LEU	159	-3.711	57.248	28.844	1.00 22.64	8
	MOTA MOTA	1302 1303	N CA	PHE PHE	160 160	-1.484 -1.430	57.396 57.576	28.855 27.409	1.00 20.79 1.00 19.10	7 6
	ATOM	1304	CB	PHE	160	-0.821	58.946	27.060	1.00 19.10	6
35	ATOM	1305	CG	PHE	160	-1.848	60.034	27.216	1.00 19.50	6
	ATOM ATOM	1306 1307		PHE	160 160	-1.971 -2.645	60.676 60.409	28.442 26.156	1.00 24.86 1.00 21.03	6 6
	ATOM	1308		PHE	160	-2.903	61.709	28.588	1.00 21.03	6
4.0	ATOM	1309		PHE	160	-3.582	61.421	26.296	1.00 19.89	6
40	ATOM ATOM	1310 1311	CZ C	PHE PHE	160 160	-3.704	62.074	27.529	1.00 25.34	6
	ATOM	1312	ŏ	PHE	160	-0.521 0.346	56.513 55.982	26.794 27.504	1.00 17.36 1.00 18.36	6 8
	MOTA	1313	N	SER	161	-0.753	56.240	25.521	1.00 17.60	7
45	atom Atom	1314 1315	CA CB	SER SER	161 161	0.087 -0.744	55.302	24.785	1.00 14.63	6 6
10	ATOM	1316	OG	SER	161	0.115	54.150 53.054	24.188 23.901	1.00 20.14 1.00 21.55	8
	ATOM	1317	С	SER	161	0.662	56.037	23.561	1.00 18.96	6
	MOTA	1318	0	SER	161	-0.101	56.753	22.894	1.00 19.79	8
50	ATOM ATOM	1319 1320	N CA	SER SER	162 162	1.921 2.518	55.796 56.404	23.232 22.049	1.00 16.19 1.00 16.74	7 6
	ATOM	1321	CB	SER	162	4.029	56.678	22.233	1.00 16.78	6
	ATOM	1322	OG	SER	162	4.801			1.00 21.00	8
	MOTA MOTA	1323 1324	С 0	SER SER	162 162	2.322 1.949	55.485 54.305	20.845 20.987	1.00 18.24 1.00 16.85	6 8
55	ATOM	1325	N	LYS	163	2.535	56.027	19.652	1.00 17.96	7
	ATOM	1326	CA	LYS	163	2.484	55.203	18.445	1.00 17.36	6
	ATOM ATOM	1327 1328	CB CG	LYS LYS	163 163	2.369 1.228	55.957 56.885	17.133 16.902	1.00 20.94 1.00 25.34	6 6
	ATOM	1329	CD	LYS	163	-0.128	56.271	16.685	1.00 29.02	6
60	ATOM	1330	CE	LYS	163	-0.954	57.131	15.721	1.00 42.35	6
	ATOM ATOM	1331 1332	NZ	LYS	163	-0.495	58.558	15.692	1.00 38.14	7
	ATOM	1333	С 0	LYS LYS	163 163	3.821 4.817	54.466 54.906	18.391 18.978	1.00 17.27 1.00 16.54	6 8
c =	ATOM	1334	N	PRO	164	3.840	53.348	17.696	1.00 18.39	7
65	ATOM	1335	CD	PRO	164	2.702	52.743	16.952	1.00 20.79	6
	ATOM ATOM	1336 1337	CA CB	PRO PRO	16 4 164	5.060 4.545	52.572 51.177	17.546 17.142	1.00 19.84 1.00 17.33	6 6
	ATOM	1338	CG	PRO	164	3.254	51.416	16.475	1.00 21.76	6
70	ATOM	1339	С	PRO	164	6.032	53.169	16.528	1.00 19.62	6
70	MOTA MOTA	1340 1341	O N	PRO VAL	164 165	5.723 7.295	53.942 52.833	15.619 16.674	1.00 19.46 1.00 17.22	8 7
		T-17	••	******	100	1.233	52.033	10.017	1.00 11.22	•

	ATOM	1342	CA	VAL	165	8.427	53.162	15.841	1.00 20.36	6
	ATOM	1343	CB	VAL	165	9.405	54.190	16.450	1.00 20.84	6
	MOTA	1344		VAL	165	10.418	54.643	15.404	1.00 20.46	6
-	MOTA	1345		VAL	165	8.699	55.475	16.899	1.00 23.72	6
5	ATOM	1346	C	VAL	165	9.173	51.833	15.590	1.00 22.05	6
	ATOM	1347	0	VAL	165	9.532	51.094	16.499	1.00 22.10 1.00 24.93	8 7
	ATOM	1348 1349	N CA	THR	166 166	9.444 10.111	51.549 50.317	14.320 13.939	1.00 24.93	6
	MOTA MOTA	1350	CB	THR	166	9.631	49.784	12.579	1.00 31.66	6
10	ATOM	1351		THR	166	9.737	50.811	11.569	1.00 38.39	8
	ATOM	1352		THR	166	8.180	49.353	12.694	1.00 23.71	6
	ATOM	1353	С	THR	166	11.611	50.597	13.909	1.00 25.06	6
	MOTA	1354	0	THR	166	11.985	51.536	13.244	1.00 21.88	8
	MOTA	1355	N	ILE	167	12.362	49.878	14.714	1.00 21.40	7
15	MOTA	1356	CA	ILE	167	13.784	49.907	14.909	1.00 25.06	6
	MOTA	1357	CB	ILE	167	14.088	50.164	16.424	1.00 26.21	6
	MOTA	1358		ILE	167	15.588	50.159	16.673	1.00 26.68 1.00 26.56	6 6
	MOTA	1359 1360		ILE	167 167	13.415 13.946	51.472 52.318	16.825 17.939	1.00 20.30	6
20	MOTA MOTA	1361	C	ILE	167	14.416	48.572	14.501	1.00 24.36	6
20	ATOM	1362	Ö	ILE	167	14.013	47.482	14.920	1.00 23.36	8
	ATOM	1363	N	THR	168	15.412	48.591	13.630	1.00 22.83	7
	ATOM	1364	CA	THR	168	16.083	47.405	13.152	1.00 27.27	6
	MOTA	1365	CB	THR	168	15.945	47.266	11.622	1.00 31.88	6
25	MOTA	1366		THR	168	14.565	47.371	11.277	1.00 32.11	8
	MOTA	1367	CG2	THR	168	16.462	45.894	11.179	1.00 34.54	6
	ATOM	1368	C	THR	168	17.575	47.414	13.501 13.508	1.00 28.53 1.00 32.64	6 8
	ATOM	1369 1370	O N	THR VAL	168 169	18.190 18.090	48.483 46.260	13.863	1.00 32.04	7
30	atom Atom	1371	CA	VAL	169	19.472	46.011	14.163	1.00 27.27	6
50	ATOM	1372	CB	VAL	169	19.728	45.359	15.523	1.00 28.51	6
	MOTA	1373		VAL	169	21.227	45.133	15.757	1.00 26.42	6
	MOTA	1374	CG2	VAL	169	19.189	46.160	16.696	1.00 27.97	6
	MOTA	1375	С	VAL	169	20.011	45.022	13.098	1.00 32.65	6
35	ATOM	1376	0	VAL	169	19.332	44.056	12.710	1.00 33.21	8
	MOTA	1377	N	GLN	170	21.245	45.196	12.689	0.01 33.85	7
	ATOM	1378	CA	GLN	170	21.966	44.390	11.737	0.01 35.75	6
	ATOM	1379	CB	GLN	170 170	23.335 24.465	44.027 44.012	12.362 11.347	0.01 36.48 0.01 37.54	6 6
40	ATOM ATOM	1380 1381	CD	GLN GLN	170	25.478	45.110	11.599	0.01 37.91	6
40	ATOM	1382		GLN	170	25.142	46.186	12.096	0.01 38.17	8
	ATOM	1383	NE2	GLN	170	26.735	44.846	11.257	0.01 38.21	7
	ATOM	1384	С	GLN	170	21.355	43.088	11.241	0.01 36.70	6
	ATOM	1385	0	GLN	170	21.049	42.167	11.995	0.01 36.81	8
45	MOTA	1386	N	VAL	171	21.273	42.959	9.919	0.01 37.51	7
	ATOM	1387	CA	VAL	171	20.781	41.772	9.240	0.01 38.20	6
	ATOM	1388	CB	VAL	171	19.483	41.208	9.842 9.681	0.01 38.61 0.01 38.88	6 6
	ATOM	1389	CG1 CG2	VAL	171 171	18.334 19.115	42.199 39.881	9.180	0.01 38.83	6
50	MOTA MOTA	1390 1391	C	VAL	171	20.587	42.048	7.750	0.01 38.42	6
50	ATOM	1392	o	VAL	171	21.420	41.573	6.949	0.01 38.53	8
	ATOM	1393	OWO		201	13.958	68.106	19.930	1.00 18.36	8
	MOTA	1394	OW0		202	13.653	41.241	23.320	1.00 24.59	8
	MOTA	1395	OW0	WAT	203	5.895	57.410	18.965	1.00 14.14	8
55	MOTA	1396	OW0		204	9.519	72.688	30.514	1.00 42.11	8
	MOTA	1397	OW0		205	8.700	64.454	28.355	1.00 21.65	8
	ATOM	1398	OW0		206	25.548	65.664	7.898	1.00 24.88 1.00 19.13	8
	ATOM	1399	OW0		207 208	2.902 14.303	52.471 45.256	31.897 23.676	1.00 19.13	8
60	MOTA MOTA	1400 1401	OW0		209	10.371	62.552	29.076	1.00 27.73	8
00	ATOM	1402	OW0		210	12.433	66.629	21.505	1.00 14.04	8
	ATOM	1403	OW0		211	5.417	47.499	21.002	1.00 16.89	8
	ATOM	1404	OW0		212	29.599	82.797	11.595	1.00 34.62	8
	ATOM	1405	OW0		213	17.813	70.187	2.648	1.00 16.34	8
65	ATOM	1406	OW0	WAT	214	6.656	58.315	16.413	1.00 24.31	8
	ATOM	1407	OW0		215	21.191	80.146	5.335	1.00 30.05	8
	ATOM	1408	OW0		216	15.621	66.766	18.319	1.00 18.82	8
	ATOM	1409	OW0		217	6.528	56.410	14.460	1.00 26.68	8
70	ATOM	1410	OW0		218	6.213	69.723	22.792 24.109	1.00 19.89 1.00 29.95	8 8
70	MOTA	1411 1412	OW0		219 220	12.935 -2.277	67.874 62.236	20.953	1.00 28.34	8
	MOTA	7.1.7.7	OM U	WVI	220					~

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	ATOM	141	3 OWO WAT	221	20.15	1 71.344	0.183	3 1.00 21.62	, ,
	ATOM				27.77				
	ATOM				-0.48				
	ATOM								
5	ATOM			225	17.81				
•	ATOM				16.60				
	ATOM			226	-0.33				
				227	13.32				
	MOTA			228	9.21		22.450	1.00 41.91	
1.0	ATOM			229	20.14	6 82.270	13.850	1.00 50.03	8
10	ATOM			230	21.70	7 80.353	12.325		
	MOTA	1423	OWO WAT	231	15.40	3 67.167	25.599		
	ATOM.	1424	OWO WAT	232	12,70				
	MOTA	1425	OWO WAT	233	12.47				8
	ATOM	142€	OWO WAT	234	13.92				
15	ATOM	1427		235	7.23				
	ATOM	1428		236	2.989				8
	ATOM	1429		237	12.86				8
	ATOM	1430		238					В
	ATOM	1431			2.754				8
20	ATOM			239	17.416				8
20		1432		240	31.068			1.00 20.85	8
	MOTA	1433		241	17.725		21.261	1.00 25.43	8
	ATOM	1434		242	32.760	65.251	6.079	1.00 38.04	8
	MOTA	1435		243	14.079	72.373	25.218	1.00 20.23	8
0.5	MOTA	1436		244	16.644	77.936	-2.315	1.00 34.00	8
25	ATOM	1437	OWO WAT	245	1.790		35.518	1.00 30.63	8
	ATOM	1438	OWO WAT	246	10.026		13.639	1.00 31.10	8
	ATOM	1439	OWO WAT	247	11.096		24.599	1.00 33.25	8
	ATOM	1440	OWO WAT	248	19.457		-2.970		
	MOTA	1441	OWO WAT	249	18.578			1.00 36.88	8
30	ATOM	1442	OWO WAT	250	11.119		26.756	1.00 30.86	8
	ATOM	1443	OWO WAT	251			16.190	1.00 37.83	8
	ATOM	1444	OWO WAT		2.583		28.032	1.00 73.18	8
	ATOM	1445	OWO WAT	252	0.243		22.803	1.00 34.15	8
				253	33.328		10.255	1.00 23.17	8
35	ATOM	1446	OWO WAT	254	22.212		5.080	1.00 51.41	8
33	ATOM	1447	OWO WAT	255	21.393		11.680	1.00 31.47	8
	ATOM	1448	OWO WAT	256	37.174	72.382	4.349	1.00 36.66	8
	ATOM	1449	OWO WAT	257	23.291	53.950	13.981	1.00 45.02	8
	MOTA	1450	OWO WAT	258	31.521	80.134	5.404	1.00 28.19	8
	ATOM	1451	OWO WAT	259	11.904	78.169	8.209	1.00 61.39	8
40	ATOM	1452	OWO WAT	260	7.393	36.160	24.668	1.00 45.96	
	ATOM	1453	OWO WAT	261	12.356	70.954	23.727		8
	ATOM	1454	OWO WAT	262	33.898	69.078		1.00 23.77	8
	ATOM	1455	OWO WAT	263	28.502		7.353	1.00 32.96	8
	ATOM	1456	OWO WAT	264		52.764	25.478	1.00 58.40	8
45	ATOM	1457			23.414	37.810	18.427	1.00 35.16	8
10			OWO WAT	265	4.792	74.631	16.778	1.00 44.49	8
	ATOM	1458	OWO WAT	266	28.509	77.721	-1.620	1.00 50.51	8
	ATOM	1459	OWO WAT	267	19.685	68.488	-0.712	1.00 45.74	8
	ATOM	1460	OWO WAT	268	10.899	74.487	23.620	1.00 43.61	8
F 0	ATOM	1461	OWO WAT	269	-1.033	73.720	20.128	1.00 34.52	8
50	MOTA	1462	OWO WAT	270	15.215	67.397	0.077	1.00 27.35	8
	ATOM	1463	OWO WAT	271	8.748	79.989	16.508	1.00 51.59	8
	MOTA	1464	OWO WAT	272	22.332	82.314	3.707	1.00 30.25	8
	MOTA	1465	OWO WAT	273	23.373	70.771	17.610	1.00 22.44	8
	ATOM	1466	OWO WAT	274	11.965	67.872	26.359	1.00 26.92	
55	MOTA	1467	OWO WAT	275	35.793	71.146	7.198		8
	ATOM	1468	OWO WAT	276	10.333			1.00 27.19	8
	ATOM	1469	OWO WAT	277		72.530	25.867	1.00 46.78	8
	ATOM	1470	OWO WAT		17.230	69.185	24.852	1.00 26.22	8
	ATOM			278	17.594	51.432	30.830	1.00 32.58	8
60		1471	OWO WAT	279	8.561	67.703	32.884	1.00 37.04	8
00	ATOM	1472	OWO WAT	280	16.374	71.765	-4.195	1.00 31.45	8
	ATOM	1473	OWO WAT	281	8.995	70.329	24.946	1.00 36.64	8
	ATOM	1474	OWO WAT	282	19.019	47.051	28.676	1.00 48.06	8
	MOTA	1475	OWO WAT	283	20.039	61.350	15.742	1.00 23.23	8
	ATOM	1476	OWO WAT	284	21.308	55.309	20.658	1.00 28.24	8
65	ATOM	1477	OWO WAT	285	7.405	70.019	5.261	1.00 41.47	8
	ATOM	1478	OWO WAT	286	23.729	66.066	0.632	1.00 30.27	
	ATOM	1479	OWO WAT	287	15.826	40.095	23.946		8
	ATOM	1480	OWO WAT	288				1.00 41.94	8
	ATOM	1481	OWO WAT		-0.119	50.371	24.812	0.50 25.93	8
70				289	3.397	54.879	42.245	1.00 29.87	8
, 0	ATOM	1482	OWO WAT	290	10.215	53.151	32.270	1.00 43.33	8
	ATOM	1483	OWO WAT	291	8.440	65.109	33.883	1.00 34.09	8

	ATOM ATOM	1		ALA ALA	401 401	-36.645 -36.199				6 6
	ATOM	3		ALA	401	-36.801				8
_	MOTA	4		ALA	401	-34.367	32.745	-3.997	1.00 45.74	7
5	MOTA MOTA	5		ALA PRO	401 402	-35.829 -35.903	32.874			6
1	ATOM	7		PRO	402	-35.149	31.367 30.320			7 6
	ATOM	8	CA.	PRO	402	-36.172	31.022			6
10	MOTA	10		PRO	402	-35.765	29.566			6
10	MOTA MOTA	10 11		PRO PRO	402 402	-34.790 -35.294	29.353 31.935			6 6
	MOTA	12		PRO	402	-34.188	32.212	-0.042	1.00 30.70	8
	ATOM	13		PRO	403	-35.789	32.370			7
15	MOTA MOTA	14 15		PRO PRO	403 403	-37.120 -35.069	32.009 33.229	2.110 2.491	1.00 35.16 1.00 38.25	6 6
	ATOM	16		PRO	403	-35.872	33.227	3.799	1.00 37.39	6
	ATOM	17		PRO	403	-37.180	32.599	3.486	1.00 37.41	6
	MOTA MOTA	18 19		PRO PRO	403 403	-33.653 -33.393	32.730	2.790	1.00 37.48	6
20	ATOM	20		LYS	404	-32.763	31.531 33.654	2.683 3.173	1.00 34.39 1.00 37.04	8 7
	ATOM	21		LYS	404	-31.399	33.188	3.424	1.00 34.97	6
	ATOM	22		LYS	404	-30.318	34.202	3.122	1.00 43.98	6
	ATOM ATOM	23 24		LYS LYS	404 404	-30.564 -29.775	35.675 36.517	3.278	1.00 47.64	6
25	ATOM	25		LYS	404	-28.317	36.123	2.292 2.137	1.00 52.03 1.00 57.56	6 6
	MOTA	26		LYS	404	-27.724	36.613	0.855	1.00 56.40	7
	MOTA	27		LYS	404	-31.243	32.632	4.825	1.00 31.44	6
	MOTA MOTA	28 29	O N	LYS ALA	404 405	-31.846 -30.416	33.097 31.586	5.784 4.908	1.00 29.91 1.00 28.75	8 7
30	MOTA	30		ALA	405	-30.039	31.053	6.218	1.00 27.21	6
	ATOM	31		ALA	405	-29.155	29.834	6.110	1.00 21.94	6
	MOTA ATOM	32 33	C	ALA ALA	405 405	-29.278 -28.760	32.183 33.072	6.923	1.00 26.42	6
	ATOM	34	N	VAL	406	-29.231	32.192	6.222 8.241	1.00 26.10 1.00 24.91	8 7
35	ATOM	35	CA	VAL	406	-28.515	33.234	8.985	1.00 26.95	6
	ATOM	36	CB	VAL	406	-29.490	34.128	9.770	1.00 29.36	6
	MOTA MOTA	37 38		VAL VAL	406 406	-28.779 -30.434	35.140 34.842	10.676 8.801	1.00 29.86 1.00 26.74	6 6
	ATOM	39	c	VAL	406	-27.503	32.613	9.942	1.00 28.93	6
40	ATOM	40	0	VAL	406	-27.846	31.872	10.866	1.00 31.46	8
	ATOM ATOM	41 42	N CA	LEU LEU	407 407	-26.233 -25.105	32.937 32.483	9.758 10.546	1.00 30.08 1.00 29.33	7 6
	ATOM	43	CB	LEU	407	-23.839	32.520	9.657	1.00 23.33	6
4 "	MOTA	44	CG	LEU	407	-22.828	31.408	9.960	1.00 34.94	6
45	ATOM ATOM	45 46		LEU LEU	407 407	-22.082	30.990	8.721	1.00 27.55	6
	MOTA	47	C	LEU	407	-21.887 -24.816	31.864 33.301	11.069 11.794	1.00 32.30 1.00 29.57	6 6
	MOTA	48	0	LEU	407	-24.653	34.515	11.800	1.00 30.04	8
50	ATOM	49	N	LYS	408	-24.768	32.624	12.930	1.00 28.04	7
30	ATOM ATOM	50 51	CA CB	LYS LYS	408 408	-24.568 -25.738	33.174 32.687	14.257 15.132	1.00 25.12 1.00 33.32	6 6
	ATOM	52	CG	LYS	408	-25.777	33.255	16.532	1.00 39.37	6
	ATOM	53	CD	LYS	408	-25.967	32.268	17.652	1.00 43.84	6
55	MOTA MOTA	54 55	CE NZ	LYS LYS	408 408	-27.129	31.305	17.487	1.00 47.78	6
30	ATOM	56	C	LYS	408	-27.525 -23.233	30.691 32.674	18.793 14.797	1.00 48.98 1.00 24.53	7 6
	ATOM	57	0	LYS	408	-22.934	31.482	14.739	1.00 25.35	8
	ATOM	58	N	LEU	409	-22.423	33.556	15.333	1.00 24.78	7
60	ATOM ATOM	59 60	CA CB	LEU LEU	409 409	-21.080 -20.189	33.313 34.383	15.843 15.190	1.00 22.07	6
	ATOM	61	CG	LEU	409	-18.725	34.503	15.596	1.00 20.04 1.00 20.57	6 6
	MOTA	62	CD1	LEU	409	-17.980	33.242	15.214	1.00 19.57	6
	ATOM ATOM	63 64	CD2		409	-18.084	35.729	14.903	1.00 23.44	6
65	atom atom	64 65	С 0	Leu Leu	409 409	-21.019 -21.424	33.451 34.473	17.346 17.869	1.00 21.01 1.00 22.38	6 8
	ATOM	66	Ň	GLU	410	-20.583	32.456	18.118	1.00 22.53	7
	ATOM	67	CA	GLU	410	-20.480	32.581	19.567	1.00 21.02	6
	atom Atom	68 69	CB	GLU	410 410	-21.523	31.684	20.270	1.00 27.36	6
70	ATOM	70	CGA CGB		410	-22.971 -22.946	32.088 32.209	20.090	0.50 28.21 0.50 38.29	6 6
	ATOM	71	CDA		410	-24.047	31.077	20.422	0.50 28.55	6

	ATOM	72		GLU	410		-23.1		33.664	20.587	0.5	0 43.48	6
	ATOM	73 74		GLU	410		-25.1		31.501			0 26.56	
	ATOM ATOM	75		GLU GLU	410 410		-22.4 -23.8		34.095 29.858	21.565 20.186		0 47.24 0 22.10	
5	ATOM	76	OE2		410		-23.8		34.380	19.908		0 46.42	8
	MOTA	77	С	GLU	410		-19.0		32.138	20.008		0 19.76	
	ATOM	78	0	GLU	410		-18.7		31.024	19.613		0 18.00	8
	MOTA MOTA	79 80	N CD	PRO PRO	411 411		-18.4		32.871	20.888		0 19.07	7
10	ATOM	81	CA	PRO	411		-17.0 -18.8		32.526 34.204	21.390 21.319		0 18.71 0 18.84	6 6
	ATOM	82	СВ	PRO	411		-17.8		34.594	22.365		17.38	6
	MOTA	83	CG	PRO	411		16.5		33.866	21.944		18.86	6
	ATOM	84	C	PRO	411		-18.7		35.108	20.090		20.01	6
15	ATOM ATOM	85 86	O N	PRO PRO	411 412		-18.3 -19.2		34.654 36.349	19.051 20.155		16.22 19.94	8 7
	ATOM	87	CD	PRO	412		19.9		36.918	21.361		21.08	6
	MOTA	88		PRO	412		19.4		37.166	18.976		20.68	6
	ATOM	89		PRO	412		20.4		38.210	19.397		19.82	6
20	MOTA MOTA	90 91		PRO PRO	412 412		20.2 18.1		38.299 37.805	20.872		23.59	6
20	ATOM	92		PRO	412		18.2		38.391	18.395 17.318		18.70 19.85	6 8
	ATOM	93		TRP	413		17.0		37.697	19.059		15.64	7
	MOTA	94		TRP	413		15.8		38.298	18.561		17.91	6
25	MOTA	95 96		TRP	413		14.6		38.026	19.562		14.32	6
23	ATOM ATOM	97	CG CD2	TRP	413 413		15.1 15.6		38.117 39.254	21.006 21.703		16.77	6
	ATOM	98	CE2		413		15.8		38.861	23.032		16.90	6 6
	ATOM	99	CE3		413		15.8		40.587	21.350		18.03	ě
30	ATOM	100	CD1		413		15.1		37.097	21.916		18.97	6
30	ATOM ATOM	101 102	NE1	TRP	413 413		15.50 16.40		37.523	23.137		11.16	7
	ATOM	103	CZ3		413		16.3		39.742 41.457	23.973 22.301		15.92 10.59	6 6
	ATOM	104	CH2		413		16.6		41.041	23.611		17.87	6
25	MOTA	105		TRP	413		15.42		37.833	17.163		19.47	6
35	ATOM	106		TRP	413		15.28		36.628	16.908		17.22	8
	ATOM ATOM	107 108		ILE ILE	414 414		15.10 14.60		38.788	16.275		16.57	7
	ATOM	109		ILE	414		15.18		38.425 39.343	14.936 13.816		18.93 16.07	6 6
• •	ATOM	110	CG2		414		16.72		39.345	13.840		16.61	6
40	ATOM	111	CG1		414		14.58		40.747	13.972		21.35	6
	ATOM ATOM	112 113	CD1	LLE	414 414		15.04		41.716	12.896		26.28	6
	ATOM	114		LLE	414		13.14 12.65		38.317 37.818	14.825 13.817		20.48 19.41	6 8
	ATOM	115		LSN	415		12.40		38.779	15.836		19.46	7
45	MOTA	116		ASN	415		10.93	35	38.596	15.778		18.11	6
	ATOM ATOM	117		ASN	415		10.16		39.904	15.731		13.53	6
	ATOM	118 119	CG A	ASN	415 415	- , - 1	10.59 11.72	Ϋ́	40.920 40.907	16.762 17.227		19.11 13.35	6
	ATOM	120	ND2 A		415		9.68		41.833	17.142		10.11	8 7
50	ATOM	121		SN	415		10.63		37.742	17.005		17.54	6
	MOTA	122		SN	415		11.01		38.131	18.111		15.32	8
	ATOM ATOM	123 124		'AL 'AL	416 416		l0.12 ·9.87		36.535	16.805		16.86	7
	ATOM	125		'AL	416		0.76		35.593 34.332	17.893 17.748		15.77 16.54	6 6
55	ATOM	126	CG1 V		416		2.25		34.725	17.733		13.42	6
	ATOM	127	CG2 V		416		0.49		33.521	16.491		18.04	6
	MOTA	128		AL	416		8.42		35.158	17.921		19.01	6
	ATOM ATOM	129 130		AL EU	416 417		7.61 8.02		35.485 34.444	17.010		17.12 17.68	8
60	ATOM	131		EU	417		6.66		33.904	18.964 19.068		15.11	7 6
	MOTA	132	CB L	EU	417		6.16		34.140	20.522		20.26	6
	ATOM	133		EU	417		5.87	3 ;	35.615	20.823	1.00	23.07	6
	ATOM	134	CD1 L		417		5.44		35.853	22.253		17.70	6
65	ATOM ATOM	135 136	CD2 L	eu Eu	417 417		4.833 6.563		36.152 32.427	19.855 18.732		26.74 16.37	6
	ATOM	137		EU	417		7.51		31.679	18.961		18.24	6 8
	ATOM	138	N G	LN	418		5.42		31.935	18.227		18.55	7
	ATOM			LN	418		5.23		30.496	18.032	1.00	19.13	6
70	ATOM			LN	418		3.790		30.145	17.696	1.00		6
, 0	ATOM ATOM			LN LN	418 418		3.510 2.120		29.617 29.964	16.314 15.800	1.00		6 6
			_ 01					. 4					-

	ATOM ATOM	143 144		1 GLN 2 GLN	418 418	-1.953 -1.135	30.834 29.248	14.943 16.333		
	ATOM	145		GLN	418	-5.561		19.348	1.00 19.43	
_	ATOM	146		GLN	418	-5.194	30.298	20.413		
5	ATOM	147		GLU	419	-6.317	28.702	19.232	1.00 19.68	
	ATOM	148	CA	GLU	419	-6.727	27.821	20.293	1.00 18.88	
	ATOM	149		GLU	419	-5.597	27.525	21.293		
	ATOM ATOM	150 151	CG CD	GLU GLU	419 419	-4.649 -3.558	26.448 26.167	20.714	1.00 30.12	6
10	ATOM	152		1 GLU	419	-3.857	25.536	21.720 22.758	1.00 41.87 1.00 48.83	6 8
	ATOM	153		2 GLU	419	-2.421	26.594	21.464	1.00 46.61	8
	ATOM	154	C	GLU	419	-8.004	28.244	20.998	1.00 21.46	
	ATOM	155	0	GLU	419	-8.496	27.461	21.815	1.00 26.39	
1 -	ATOM	156	N	ASP	420	-8.606	29.360	20.619	1.00 19.91	7
15	ATOM	157	CA	ASP	420	-9.898	29.772	21.114	1.00 20.76	6
	MOTA MOTA	158 159	CB CG	ASP ASP	420 420	-10.285 -9.587	31.217 32.288	20.726 21.526	1.00 13.47	6
	ATOM	160		LASP	420	-8.873	32.260	22.534	1.00 13.93 1.00 17.57	6 8
	MOTA	161		ASP	420	-9.723	33.461	21.104	1.00 13.79	8
20	MOTA	162	C	ASP	420	-11.002	28.916	20.451	1.00 19.58	6
	MOTA	163	0	ASP	420	-10.913	28.647	19.262	1.00 17.49	8
	MOTA	164	N	SER	421	-12.071	28.668	21.174	1.00 17.22	7
	ATOM ATOM	165 166	CA	SER SER	421	-13.233	27.937	20.659	1.00 17.62	6
25	ATOM	167		SER	421 421	-14.011 -13.981	27.341 27.310	21.844 21.846	0.50 17.49 0.50 13.14	6 6
	ATOM	168		SER	421	-14.900	26.350	21.355	0.50 22.95	8
	MOTA	169		SER	421	-13.175	26.287	22.416	0.50 6.85	8
	MOTA	170	С	SER	421	-14.181	28.828	19.873	1.00 18.61	6
20	ATOM	171	0	SER	421	-14.424	29.982	20.265	1.00 21.41	8
30	ATOM	172	N	VAL	422	-14.638	28.354	18.721	1.00 15.80	7
	ATOM ATOM	173 174	CA CB	VAL VAL	422 422	-15.585 -15.052	29.133 29.632	17.910 16.560	1.00 17.93 1.00 20.37	6 6
	ATOM	175		VAL	422	-16.093	30.465	15.804	1.00 20.37	6
	ATOM	176		VAL	422	-13.858	30.566	16.679	1.00 17.26	6
35	MOTA	177	C	VAL	422	-16.822	28.257	17.665	1.00 19.20	6
	MOTA	178	0	VAL	422	-16.633	27.097	17.291	1.00 18.52	8
	ATOM	179	N	THR	423	-18.021	28.759	17.917	1.00 16.32	7
	ATOM ATOM	180 181	CA CB	THR THR	423 423	-19.249 -20.080	28.043 27.738	17.648 18.911	1.00 19.99 1.00 22.97	6 6
40	ATOM	182		THR	423	-19.192	27.117	19.850	1.00 22.37	8
	MOTA	183	CG2		423	-21.241	26.809	18.614	1.00 16.78	6
	MOTA	184	С	THR	423	-20.098	28.850	16.658	1.00 24.68	6
	ATOM	185	0	THR	423	-20.509	29.986	16.897	1.00 22.59	8
45	ATOM	186	N	LEU	424	-20.257	28.248	15.467	1.00 23.73	7
43	MOTA MOTA	187 188	CA CB	LEU LEU	424 424	-21.081 -20.427	28.815	14.423	1.00 23.11	6 6
	ATOM	189	CG	LEU	424	-19.053	28.660 29.386	13.046 12.959	1.00 20.25 1.00 23.95	6
	ATOM	190		LEU	424	-18.324	29.010	11.681	1.00 20.78	6
	ATOM	191	CD2	LEU	424	-19.251	30.881	13.049	1.00 22.74	6
50	MOTA	192	С	LEU	424	-22.444	28.103	14.450	1.00 25.87	6
	ATOM	193	0	LEU	424	-22.470	26.858	14.537	1.00 24.57	8
	ATOM ATOM	194 195	N CA	THR THR	425 425	-23.520 -24.847	28.886 28.266	14.367 14.336	1.00 20.22 1.00 23.21	7
	ATOM	196	CB	THR	425	-25.656	28.601	15.597	1.00 23.21	6 6
55	MOTA	197	OG1		425	-24.945	28.136	16.755	1.00 26.30	8
	MOTA	198	CG2		425	-27.041	27.941	15.590	1.00 28.49	6
	MOTA	199	C	THR	425	-25.604	28.700	13.075	1.00 22.31	6
	ATOM	200	0	THR	425	-25.706	29.915	12.819	1.00 23.86	8
60	ATOM ATOM	201 202	N	CYS	426 426	-26.092 -26.832	27.732	12.307	1.00 18.68	7
00	ATOM	202	CA C	CYS CYS	426	-28.345	27.978 27.956	11.075 11.346	1.00 23.20 1.00 23.06	6 6
	ATOM	204	ŏ	CYS	426	-28.957	26.886	11.556	1.00 23.76	8
	ATOM	205	CB	CYS	426	-26.509	26.985	9.958	1.00 17.92	6
C.E.	ATOM	206	SG	CYS	426	-27.138	27.508	8.311	1.00 22.25	16
65	ATOM	207	N	GLN	427	-28.929	29.137	11.355	1.00 19.35	7
	MOTA MOTA	208 209	CA CB	GLN GLN	427 427	-30.332 -30.543	29.345	11.658	1.00 23.30 1.00 29.78	6
	ATOM	210	CG	GLN	427	-29.623	30.657 30.822	12.464 13.672	1.00 29.78	6 6
	ATOM	211	CD	GLN	427	-29.927	32.038	14.518	1.00 31.30	6
70	MOTA	212	OE1		427	-30.322	33.092	14.032	1.00 38.67	8
	ATOM	213	NE2	GLN	427	-29.792	31.971	15.834	1.00 36.36	7

	B m cohr	214	C	GLN	427	-31.169	29.449	10.377	1.00 26.33	6
	ATOM								1.00 23.15	
	ATOM	215	0	GLN	427	-30.764	30.010	9.347		8
	MOTA	216	N	GLY	428	-32.363	28.847	10.438	1.00 27.69	7
	ATOM	217	CA	GLY	428	-33.289	28.847	9.313	1.00 28.02	6
5	ATOM	218	c	GLY	428	-34.022	27.506	9.215	1.00 29.41	6
J									1.00 28.46	8
	ATOM	219	0	GLY	428	-33.639	26.531	9.862		
	MOTA	220	N	ALA	429	-35.062	27.445	8.389	1.00 27.48	7
	MOTA	221	CA	ALA	429	-35.824	26.226	8.210	1.00 27.39	6
	ATOM	222	CB	ALA	429	-36.979	26.513	7.239	1.00 25.91	6
1.0										6
10	MOTA	223	С	ALA	429	-34.959	25.136	7.574	1.00 28.27	
	ATOM	224	0	ALA	429	-34.315	25.451	6.561	1.00 26.07	8
	ATOM	225	N	ARG	430	-35.060	23.915	8.064	1.00 23.97	7
	ATOM	226	CA	ARG	430	-34.303	22.811	7.490	1.00 27.17	6
				ARG	430	-33.571	22.043	8.601	1.00 30.34	6
- F	MOTA	227	CB							
15	ATOM	228	CG	ARG	430	-32.574	22.776	9.460	1.00 34.05	6
	MOTA	229	CD	ARG	430	-32.365	21.986	10.761	1.00 33.86	6
	MOTA	230	NE	ARG	430	-32.407	22.964	11.836	1.00 38.60	7
	ATOM	231	CZ	ARG	430	-32.487	22.784	13.126	1.00 38.08	6
										7
	MOTA	232		ARG	430	-32.567	21.568	13.635	1.00 36.51	
20	MOTA	233	NH2	ARG	430	-32.467	23.876	13.879	1.00 46.13	7
	MOTA	234	С	ARG	430	-35.194	21.718	6.880	1.00 26.70	6
	ATOM	235	ō	ARG	430	-36.399	21.724	7.075	1.00 29.22	8
										7
	MOTA	236	N	SER	431	-34.573	20.737	6.246	1.00 26.85	
	ATOM	237	CA	SER	431	-35.315	19.582	5.738	1.00 26.56	6
25	ATOM	238	CB	SER	431	-34.682	19.020	4.476	1.00 25.03	6
	ATOM	239	OG	SER	431	-34.562	19.991	3.477	1.00 27.59	8
									1.00 26.58	6
	MOTA	240	С	SER	431	-35.273	18.545	6.861		
	MOTA	241	0	SER	431	-34.396	18.620	7.739	1.00 23.91	8
	ATOM	242	N	PRO	432	-36.163	17.558	6.839	1.00 23.48	7
30	ATOM	243	CD	PRO	432	-37.224	17.383	5.842	1.00 22.70	6
30						-36.176	16.516	7.861	1.00 24.75	6
	MOTA	244	CA.	PRO	432					
	MOTA	245	CB	PRO	432	-37.621	16.036	7.805	1.00 24.34	6
	MOTA	246	CG	PRO	432	-38.095	16.295	6.414	1.00 23.77	6
	ATOM	247	С	PRO	432	-35.172	15.417	7.549	1.00 29.23	6
35		248	ō	PRO	432	-35.472	14.257	7.223	1.00 28.28	8
33	ATOM									
	ATOM	249	N	GLU	433	-33.913	15.745	7.709	1.00 29.77	7
	MOTA	250	CA	GLU	433	-32.725	14.970	7.417	1.00 33.37	6
	MOTA	251	CBA	GLU	433	-32.177	15.440	6.073	0.50 35.18	6
	ATOM	252		GLU	433	-32.123	15.409	6.084	0.50 31.98	6
4.0									0.50 39.40	6
40	ATOM	253		GLU	433	-30.795	16.037	5.952		
	MOTA	254	CGB	GLU	433	-31.776	16.876	5.954	0.50 34.05	6
	MOTA	255	CDA	GLU	433	-30.394	16.341	4.521	0.50 46.48	6
	ATOM	256	CDB	GLU	433	-31.601	17.333	4.517	0.50 34.67	6
	ATOM	257		GLU	433	-29.268	16.010	4.076	0.50 49.23	8
AE									0.50 32.81	8
45	ATOM	258		GLU	433	-32.194	16.698	3.619		
	MOTA	259	OE2	GLU	433	-31.232	16.914	3.788	0.50 47.50	8
	ATOM	260	OE2	GLU	433	-30.877	18.324	4.275	0.50 24.64	8
	ATOM	261	С	GLU	433	-31.683	15.177	8.519	1.00 32.61	6
				GLU	433	-31.612	16.266	9.085	1.00 28.72	8
r 0	ATOM	262	0							
50	ATOM	263	N	SER	434	-30.844	14.184	8.743	1.00 32.15	7
	ATOM	264	CA	SER	434	-29.804	14.275	9.764	1.00 32.72	6
	ATOM	265	CB	SER	434	-29.277	12.853	10.037	1.00 34.26	6
	ATOM	266	OG	SER	434	-28.320	12.935	11.093	1.00 45.88	8
								9.332		
	MOTA	267	С	SER	434	-28.668	15.192		1.00 30.93	6
55	ATOM	268	0	SER	434	-28.156	15.983	10.124	1.00 28.87	8
	ATOM	269	N	ASP	435	-28.222	15.093	8.082	1.00 28.02	7
	MOTA	270	CA	ASP	435	-27.167	16.008	7.599	1.00 28.62	6
									1.00 29.65	6
	MOTA	271	CB	ASP	435	-26.292	15.328	6.585		0
	MOTA	272	CG	ASP	435	-25.357	14.227	7.057	1.00 37.43	6
6 0	MOTA	273	OD1	ASP	435	-25.027	14.097	8.258	1.00 33.53	8
* -	ATOM	274		ASP	435	-24.902	13.470	6.154	1.00 36.01	8
							17.223	6.973	1.00 27.08	6
	ATOM	275	С	ASP	435	-27.882				
	ATOM	276	0	ASP	435	-27.997	17.300	5.756	1.00 28.07	8
	MOTA	277	N	SER	436	-28.461	18.118	7.774	1.00 25.55	7
65	ATOM	278	CA	SER	436	-29.282	19.186	7.225	1.00 27.45	6
				SER	436	-30.440	19.435	8.213	1.00 34.87	6
	MOTA	279	CB						1.00 39.51	
	MOTA	280	OG	SER	436	-29.973	20.064	9.405		8
	ATOM	281	С	SER	436	-28.558	20.484	6.890	1.00 27.14	6
	ATOM	282	0	SER	436	-29.143	21.445	6.363	1.00 25.67	8
70		283	N	ILE	437	-27.293	20.643	7.231	1.00 24.64	7
, 0	ATOM								1.00 24.33	6
	MOTA	284	CA	ILE	437	-26.580	21.893	6.977	1.00 44.33	J

	ATOM ATOM ATOM	286 CG2 ILE	437	-26.164 22.559 8.309 1.00 30.71 6 -25.561 23.935 8.032 1.00 26.94 6 -27.333 22.645 9.308 1.00 21.66 6
5	ATOM ATOM ATOM	288 CD1 ILE 289 C ILE 290 O ILE	437 437 437	-27.333 22.645 9.308 1.00 21.66 6 -28.443 23.588 8.867 1.00 27.66 6 -25.336 21.707 6.128 1.00 24.08 6 -24.515 20.833 6.390 1.00 23.50 8
10	ATOM ATOM ATOM ATOM	292 CA GLN 293 CB GLN		-25.122 22.552 5.127 1.00 24.52 7 -23.862 22.570 4.399 1.00 23.13 6 -24.016 22.798 2.905 1.00 29.28 6
	ATOM ATOM ATOM	295 CD GLN 296 OE1 GLN 297 NE2 GLN	438 438 438	-24.458 21.570 2.123 1.00 29.86 6 -24.692 21.901 0.661 1.00 33.48 6 -25.540 22.744 0.323 1.00 28.34 8 -23.922 21.198 -0.177 1.00 38.54 7
15	MOTA MOTA MOTA	298 C GLN 299 O GLN 300 N TRP 301 CA TRP	438 438 439 439	-23.048 23.738 4.985 1.00 23.81 6 -23.598 24.844 5.087 1.00 22.62 8 -21.807 23.480 5.371 1.00 21.43 7
20	ATOM ATOM ATOM ATOM	302 CB TRP 303 CG TRP 304 CD2 TRP 305 CE2 TRP	439 439 439	-20.345 24.233 7.257 1.00 21.01 6 -21.264 24.233 8.430 1.00 17.58 6 -21.721 25.343 9.212 1.00 17.00 6
2.5	ATOM ATOM ATOM	306 CE3 TRP 307 CD1 TRP 308 NE1 TRP	439 439 439 439	-22.569 24.833 10.220 1.00 16.71 6 -21.495 26.719 9.158 1.00 21.47 6 -21.844 23.116 8.974 1.00 19.92 6 -22.626 23.466 10.061 1.00 22.18 7
25	ATOM ATOM ATOM ATOM	309 CZ2 TRP 310 CZ3 TRP 311 CH2 TRP 312 C TRP	439 439 439 439	-23.218 25.646 11.152 1.00 18.29 6 -22.109 27.537 10.091 1.00 21.62 6 -22.960 26.992 11.064 1.00 20.15 6
30	ATOM ATOM ATOM ATOM	313 O TRP 314 N PHE 315 CA PHE	439 440 440	-19.407 23.941 4.238 1.00 23.42 8 -19.533 26.165 4.758 1.00 22.91 7 -18.512 26.477 3.754 1.00 26.86 6
35	ATOM ATOM MOTA	316 CB PHE 317 CG PHE 318 CD1 PHE 319 CD2 PHE	440 440 440 440	-19.121 27.144 2.513 1.00 24.16 6 -20.225 26.437 1.788 1.00 23.96 6 -21.551 26.586 2.189 1.00 23.61 6
	ATOM ATOM ATOM ATOM	320 CE1 PHE 321 CE2 PHE 322 CZ PHE 323 C PHE	440 440 440 440	-22.564 25.947 1.504 1.00 20.83 6 -20.967 24.986 0.020 1.00 21.69 6 -22.267 25.126 0.432 1.00 21.86 6
40	ATOM ATOM ATOM	324 O PHE 325 N HIS 326 CA HIS	440 441 441	-17.466 27.431 4.349 1.00 23.51 6 -17.838 28.278 5.151 1.00 21.94 8 -16.232 27.291 3.905 1.00 21.59 7 -15.107 28.095 4.366 1.00 24.07 6
45	ATOM ATOM ATOM ATOM	327 CB HIS 328 CG HIS 329 CD2 HIS 330 ND1 HIS	441 441 441 441	-14.032 27.294 5.099 1.00 18.72 6 -12.864 28.139 5.548 1.00 23.41 6 -12.794 29.451 5.899 1.00 21.85 6
50	ATOM ATOM ATOM ATOM	331 CE1 HIS 332 NE2 HIS 333 C HIS	441 441 441	-10.789 28.607 6.135 1.00 22.79 6 -11.504 29.705 6.268 1.00 21.87 7 -14.455 28.703 3.115 1.00 21.83 6
30	ATOM ATOM ATOM	334 O HIS 335 N ASN 336 CA ASN 337 CB ASN	441 442 442 442	-13.972 27.947 2.282 1.00 21.37 8 -14.576 30.019 2.959 1.00 22.08 7 -14.077 30.670 1.726 1.00 20.46 6
55	ATOM ATOM ATOM ATOM	338 CG ASN 339 OD1 ASN 340 ND2 ASN	442 442 442	-11.925 31.469 2.761 1.00 22.74 6 -12.473 32.523 3.087 1.00 24.40 8 -10.804 31.062 3.341 1.00 18.43 7
60	ATOM ATOM ATOM		442 442 443 443	-14.733 30.055 0.488 1.00 21.32 6 -14.085 29.819 -0.533 1.00 20.13 8 -16.002 29.646 0.568 1.00 20.53 7
	ATOM MOTA ATOM MOTA	345 C GLY 346 O GLY 347 N ASN	443 443 444	-16.586 27.506 -0.661 1.00 24.51 6 -17.209 26.879 -1.550 1.00 25.30 8 -15.633 26.896 0.051 1.00 21.27 7
65	ATOM ATOM ATOM	349 CB ASN 350 CG ASN 351 OD1 ASN	444 444 444 444	-15.391 25.473 -0.112 1.00 20.46 6 -13.903 25.132 0.000 1.00 23.82 6 -13.049 26.032 -0.891 1.00 22.26 6
70	ATOM ATOM ATOM ATOM	353 C ASN 4	444 444 144 145	-12.146 26.722 -0.409 1.00 25.47 8 -13.382 26.079 -2.171 1.00 21.59 7 -16.208 24.723 0.937 1.00 19.78 6 -16.180 25.088 2.107 1.00 22.07 8 -16.907 23.678 0.523 1.00 22.22 7

5	OTA OTA OTA OTA OTA OTA	M 357 CB LEU M 358 CG LEU M 359 CD1 LEU M 360 CD2 LEU M 361 C LEU	445 -17.730 22.904 1.459 1.00 21.67 6 445 -18.391 21.725 0.715 1.00 28.15 6 445 -19.159 20.695 1.538 1.00 29.14 6 445 -20.479 21.295 2.002 1.00 25.07 6 445 -19.452 19.400 0.775 1.00 28.51 6 445 -16.825 22.307 2.525 1.00 22.27 6 445 -15.748 21.860 2.525 1.00 22.27 6
10	ATOM ATOM ATOM ATOM ATOM	1 363 N ILE 4 1 364 CA ILE 4 1 365 CB ILE 4 366 CG2 ILE 4	146 -17.263 22.262 3.766 1.00 20.11 7 146 -16.539 21.544 4.835 1.00 24.64 6 146 -16.657 22.358 6.132 1.00 22.24 6 146 -16.007 21.732 7.358 1.00 21.33 6
15	ATOM ATOM ATOM ATOM ATOM	368 CD1 ILE 4 369 C ILE 4 370 O ILE 4 371 N PRO 4	46 -16.664 24.719 7.024 1.00 20.74 6 46 -17.351 20.241 5.066 1.00 25.53 6 46 -18.419 20.266 5.624 1.00 22.91 8 47 -16.937 19.119 4.444 1.00 30.56
20	ATOM ATOM ATOM ATOM ATOM	373 CA PRO 44 374 CB PRO 44 375 CG PRO 44 376 C PRO 44	17.731 17.898 4.434 1.00 32.61 6 17.731 17.898 4.434 1.00 30.93 6 17.1030 17.030 3.363 1.00 31.28 6 17.1046 3.441 1.00 32.54 6 17.10488 17.104 5.706 1.00 32.54 6
25	ATOM ATOM ATOM ATOM ATOM	378 N THR 44 379 CA THR 44 380 CB THR 44 381 OG1 THR 44	-18.733 16.196 5.747 1.00 29.24 8 -17.092 17.353 6.730 1.00 26.79 7 -17.135 16.568 7.971 1.00 26.97 6 8 -15.698 16.543 8.532 1.00 31.78 6 8 -15.241 17.908 8.520 1.00 31.45
30	ATOM ATOM ATOM ATOM ATOM	383 C THR 44 384 O THR 44 385 N HIS 44 386 CA HIS 44	-14.798 15.716 7.605 1.00 27.40 6 -18.075 17.109 9.021 1.00 26.31 6 -18.206 16.532 10.113 1.00 28.00 8 -18.698 18.264 8.772 1.00 24.44 7 -19.612 18.924 9.707 1.00 24.44 7
35	ATOM ATOM ATOM ATOM ATOM	388 CG HIS 449 389 CD2 HIS 449 390 ND1 HIS 449 391 CE1 HIS 449	-18.953 20.256 10.174 1.00 25.11 6 -17.722 19.927 10.961 1.00 22.20 6 -16.430 19.757 10.624 1.00 27.86 6 -17.809 19.641 12.306 1.00 29.80 7 -16.595 19.340 12.363 1.00 29.80 7
40	ATOM ATOM ATOM ATOM	392 NE2 HIS 449 393 C HIS 449 394 O HIS 449 395 N THR 450 396 CA THR 450	-15.748 19.392 11.761 1.00 25.35 7 -20.923 19.278 9.041 1.00 23.08 6 -20.942 20.061 8.075 1.00 20.57 8 -22.038 18.704 9.497 1.00 25.11 7
45	ATOM ATOM ATOM ATOM ATOM	397 CB THR 450 398 OG1 THR 450 399 CG2 THR 450 400 C THR 450 401 O THR 450	-23.732 17.552 8.807 1.00 22.98 6 -23.843 16.614 9.231 1.00 23.01 6 -22.757 17.049 7.101 1.00 19.07 6 -24.460 19.221 9.766 1.00 24.61 6
50	ATOM ATOM ATOM ATOM ATOM	402 N GLN 451 403 CA GLN 451 404 CB GLN 451 405 CG GLN 451	-24.126 19.592 10.985 1.00 24.52 7 -25.132 19.887 11.995 1.00 27.31 6 -24.708 19.361 13.378 1.00 28.63 6 -24.438 17.852 13.378 1.00 28.63
55	ATOM ATOM ATOM ATOM	407 OE1 GLN 451 408 NE2 GLN 451 409 C GLN 451 410 O GLN 451	-25.677 17.056 12.995 1.00 38.53 6 -26.606 16.914 13.802 1.00 37.60 8 -25.724 16.535 11.765 1.00 32.79 7 -25.411 21.379 12.101 1.00 26.69 6
60	ATOM ATOM ATOM ATOM ATOM	411 N PRO 452 412 CD PRO 452 413 CA PRO 452 414 CB PRO 452 415 CG PRO 452	-26.510 21.728 12.769 1.00 25.16 7 -27.553 20.775 13.270 1.00 24.54 6 -26.917 23.103 12.974 1.00 25.24 6 -28.264 22.978 13.708 1.00 26.09 6
65	MOTA	416 C PRO 452 417 O PRO 452 418 N SER 453 419 CA SER 453 420 CB SER 453	-25.900 23.951 13.722 1.00 25.71 6 -25.877 25.179 13.542 1.00 25.71 6 -25.044 23.369 14.556 1.00 24.05 7 -23.991 24.093 15.239 1.00 25.63 6
70	ATOM ATOM ATOM ATOM ATOM	421 OG SER 453 422 C SER 453 423 O SER 453 424 N TYR 454 425 CA TYR 454 426 CB TYR 454	-24.105

	ATOM	427	CG	TYR	454	-18.612	23.868	12.274	1.00 30.15	6
	ATOM ATOM	428 429		L TYR	454 454	-17.719 -16.407	22.961 22.860	12.825 12.409	1.00 29.18 1.00 31.26	6 6
	ATOM	430		TYR	454	-18.104	24.700	11.280	1.00 31.20	6
5	ATOM	431		TYR	454	-16.796	24.649	10.855	1.00 31.66	6
	ATOM	432	CZ	TYR	454	-15.950	23.715	11.429	1.00 33.63	6
	ATOM	433	OH	TYR	454	-14.624	23.647	11.038	1.00 34.53	8
	MOTA	434	C	TYR	454	-19.378	24.416	15.167	1.00 24.84	6
10	ATOM ATOM	435 436	O N	TYR ARG	454 455	-19.300 -18.773	25.656 23.685	15.129 16.070	1.00 22.53 1.00 21.66	8 7
10	ATOM	437	CA	ARG	455	-17.864	24.216	17.070	1.00 23.60	6
	MOTA	438	CB	ARG	455	-18.242	23.709	18.480	1.00 25.95	6
	MOTA	439	CG	ARG	455	-17.478	24.526	19.551	1.00 23.98	6
1.5	MOTA	440	CD	ARG	455	-17.651	23.884	20.918	1.00 35.38	6
15	MOTA	441	NE CZ	ARG	455	-16.821	24.501	21.956	1.00 27.47	7
	ATOM ATOM	442 443		ARG ARG	455 455	-17.278 -18.570	25.336 25.657	22.879 22.904	1.00 33.10 1.00 30.00	6 7
	MOTA	444		ARG	455	-16.418	25.817	23.778	1.00 30.00	7
	MOTA	445	С	ARG	455	-16.434	23.763	16.802	1.00 27.49	6
20	MOTA	446	0	ARG	455	-16.275	22.554	16.569	1.00 22.62	8
	MOTA	447	N	PHE	456	-15.455	24.692	16.781	1.00 23.78	7
	ATOM	448	CA	PHE	456	-14.092	24.230	16.510	1.00 21.92	6
	MOTA MOTA	449 450	CB CG	PHE	456 456	-13.716 -13.819	24.371 25.735	15.036 14.386	1.00 25.99 1.00 20.84	6 6
25	ATOM	451		PHE	456	-15.019	26.213	13.897	1.00 20.84	6
	ATOM	452	CD2		456	-12.705	26.547	14.264	1.00 20.31	6
	ATOM	453	CE1	PHE	456	-15.103	27.451	13.283	1.00 21.52	6
	ATOM	454	CE2		456	-12.768	27.789	13.680	1.00 18.36	6
30	MOTA	455	CZ	PHE	456	-13.973	28.250	13.159	1.00 18.38	6
30	MOTA MOTA	456 457	С 0	PHE	456 456	-13.095 -13.454	25.004 26.033	17.372 17.921	1.00 23.93 1.00 22.42	6 8
	ATOM	458	N	LYS	457	-11.865	24.526	17.423	1.00 22.42	7
	MOTA	459	CA	LYS	457	-10.735	25.207	18.054	1.00 24.34	6
	ATOM	460	CBA	LYS	457	-9.892	24.246	18.881	0.50 28.51	6
35	ATOM	461		LYS	457	-9.822	24.139	18.669	0.50 22.87	6
	MOTA	462		LYS	457	-10.656	23.568	20.010	0.50 33.64	6
	atom atom	463 464		LYS	457 457	-8.769 -11.436	24.658 24.524	19.632 20.892	0.50 24.29 0.50 40.75	6 6
	ATOM	465		LYS	457	-8.631	23.680	20.798	0.50 26.90	6
40	MOTA	466		LYS	457	-12.612	23.876	21.603	0.50 43.07	6
	ATOM	467		LYS	457	-9.138	24.262	22.092	0.50 29.79	6
	MOTA	468		LYS	457	-12.703	24.236	23.044	0.50 51.71	7
	ATOM ATOM	469 470	C	LYS LYS	457 457	-8.050 -9.950	24.601 25.943	23.060 16.969	0.50 36.22 1.00 21.30	7 6
45	ATOM	471	ō	LYS	457	-9.436	25.315	16.052	1.00 21.30	8
	ATOM	472	N	ALA	458	-9.928	27.278	16.945	1.00 18.23	7
	ATOM	473	CA	ALA	458	-9.341	28.002	15.821	1.00 15.74	6
	ATOM	474	CB	ALA	458	-9.612	29.505	16.094	1.00 9.09	6
50	ATOM	475	C	ALA	458	-7.841	27.832	15.614	1.00 20.26	6
50	MOTA MOTA	476 477	o N	ALA ASN	458 459	-7.067 -7.392	27.802 27.740	16.574 14.367	1.00 18.04 1.00 18.31	8 7
	ATOM	478	CA	ASN	459	-5.986	27.795	14.019	1.00 23.04	6
	ATOM	479	СВ	ASN	459	-5.222	26.565	13.612	1.00 32.39	6
	MOTA	480	CG	ASN	459	-5.880	25.223	13.665	1.00 38.26	6
55	ATOM	481		ASN	459	-5.855	24.587	14.716	1.00 42.50	8
	MOTA	482		ASN	459	-6.426	24.800	12.529	1.00 43.39	7
	ATOM ATOM	483 484	С 0	asn asn	459 459	-5.825 -6.794	28.814 29.390	12.867 12.365	1.00 24.07 1.00 21.25	6 8
	MOTA	485	N	ASN	460	-4.582	29.033	12.484	1.00 24.40	7
60	ATOM	486	CA	ASN	460	-4.192	30.043	11.519	1.00 31.47	6
	ATOM	487	CB	ASN	460	-2.680	29.973	11.234	1.00 31.46	6
	ATOM	488	CGA		460	-2.272	31.090	10.274	0.50 31.26	6
	ATOM	489	CGB		460	-2.221	28.594	10.814	0.50 35.72	6
65	ATOM ATOM	490 491	OD1		460 460	-2.337 -2.985	32.284 27.626	10.597 10.768	0.50 22.52 0.50 33.04	8 8
J J	ATOM	492	ND2		460	-1.863	30.691	9.070	0.50 26.04	7
	ATOM	493	ND2		460	-0.932	28.475	10.483	0.50 39.47	7
	ATOM	494	С	ASN	460	-5.006	29.923	10.234	1.00 29.05	6
7.0	MOTA	495	0	ASN	460	-5.645	30.880	9.780	1.00 32.27	8
70	MOTA	496	N	ASN	461	-5.098	28.713	9.710	1.00 30.20	7
	ATOM	497	CAA	ASN	461	-5.863	28.379	8.529	0.50 28.68	6

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	499 CBA ASN 500 CBB ASN 501 CGA ASN 502 CGB ASN 503 OD1 ASN	461 461 461 461	-5.857 -5.564 -5.403 -4.101 -5.608 -3.502 -6.383	28.499 26.911 27.195 26.739 25.984 25.741	8.477 8.150 7.806 7.792 8.678 8.184	0.50 29.13 0.50 26.19 0.50 30.25 0.50 27.01 0.50 32.36 0.50 28.58	6 6 6 6 8
10	ATOM ATOM ATOM ATOM ATOM	505 ND2 ASN 506 ND2 ASN 507 C ASN 508 O ASN 509 N ASP	461 461 461 461 462	-3.526 -4.927 -7.371 -8.030 -7.932	26.046 27.694 24.875 28.530 28.331 28.888	9.637 7.071 8.384 8.628 7.617 9.767	0.50 33.38 0.50 34.39 0.50 33.52 1.00 25.33 1.00 21.46 1.00 24.89	8 7 7 6 8 7
15	ATOM ATOM ATOM ATOM ATOM ATOM	510 CA ASP 511 CB ASP 512 CG ASP 513 OD1 ASP 514 OD2 ASP	462 462 462 462 462	-9.276	29.024 28.582 27.084 26.317 26.593	9.941 11.372 11.538 10.570 12.611	1.00 21.37 1.00 16.89 1.00 26.20 1.00 20.81 1.00 17.90	6 6 6 8
20	ATOM ATOM ATOM ATOM ATOM	515 C ASP 516 O ASP 517 N SER 518 CA SER 519 CB SER 520 OG SER	462 462 463 463 463 463	-11.104 -9.011 -9.434 -8.268	30.427 30.657 31.389 32.734 33.702	9.645 9.654 9.394 9.015 8.811	1.00 18.69 1.00 20.50 1.00 19.81 1.00 19.84 1.00 22.04	6 8 7 6
25	ATOM ATOM ATOM ATOM ATOM	521 C SER 522 O SER 523 N GLY 524 CA GLY 525 C GLY	463 463 464 464 464	-10.196 -10.015 -11.056 -11.769	33.848 32.662 31.706 33.671 33.675	10.009 7.682 6.911 7.467 6.190	1.00 20.02 1.00 23.89 1.00 17.92 1.00 19.50 1.00 22.23	8 6 8 7 6
30	ATOM ATOM ATOM ATOM ATOM	526 O GLY 527 N GLU 528 CA GLU 529 CBA GLU 530 CBB GLU	464 465 465 465 465	-13.744 3 -13.980 3 -15.428 3 -15.934 3	33.901 34.302 33.640 33.853 34.304	6.340 7.399 5.238 5.269 3.901	1.00 19.81 1.00 18.93 1.00 17.01 1.00 21.39 0.50 13.64	6 8 7 6
35	ATOM ATOM ATOM ATOM ATOM	531 CGA GLU 532 CGB GLU 533 CDA GLU 534 CDB GLU 535 OE1 GLU	465 465 465 465 465	-16.507 3 -15.409 3 -16.656 3 -15.898 3	35.708 35.807 36.187 36.901	3.813 3.602 2.381 4.520	0.50 23.81 0.50 15.71 0.50 32.15 0.50 22.33 0.50 40.56	6 6 6
40	ATOM ATOM ATOM ATOM ATOM	536 OE1 GLU 537 OE2 GLU 538 OE2 GLU 539 C GLU 540 O GLU	465 465 465 465 465	-16.578 3 -15.991 3 -15.624 3 -16.155 3	5.603 6.595 7.180 8.108 2.542	5.525 2.014 4.278 5.593	0.50 22.70 0.50 41.83 0.50 31.04 0.50 46.02 1.00 21.56	8 8 8 8
45	ATOM ATOM ATOM ATOM ATOM	541 N TYR 542 CA TYR 543 CB TYR 544 CG TYR 545 CD1 TYR	466 466 466 466 466	-17.172 3: -17.966 3: -17.954 3: -16.620 3:	1.541 2.598 1.383 0.882	6.458 1 6.691 1 8.129 1 8.534 1	1.00 21.41 1.00 21.38 1.00 17.91 1.00 17.39 1.00 18.08	8 7 6 6 6
50	ATOM ATOM ATOM ATOM ATOM	546 CE1 TYR 547 CD2 TYR 548 CE2 TYR 549 CZ TYR 550 OH TYR	466 466 466 466 466	-14.369 30 -16.348 28 -15.102 28 -14.124 29		9.323 1 8.485 1 8.867 1 9.279 1	1.00 16.48 1.00 18.23 1.00 18.37 1.00 18.98	6 6 6 6
55	ATOM ATOM ATOM ATOM ATOM	551 C TYR 552 O TYR 553 N THR 554 CA THR	466 466 467 467	-19.379 31 -19.923 32 -20.010 30 -21.374 30	. 635 . 731 . 638 . 728	6.212 1 6.353 1 5.568 1 5.117 1	.00 13.96 .00 18.14 .00 17.95	8 6 8 7 6
60	ATOM ATOM ATOM ATOM ATOM	556 OG1 THR 557 CG2 THR 558 C THR 559 O THR	467 467 467 467	-20.669 30 -21.215 32 -22.044 29 -21.354 28	.129 .495 .358	2.835 1 3.309 1 5.384 1	.00 22.52 6 .00 16.85 8 .00 17.46 6 .00 18.76 6	5
65	ATOM ATOM ATOM ATOM	561 CA CYS 562 C CYS 563 O CYS 564 CB CYS	468 468 468 468 468	-23.354 29 -24.099 28 -25.382 28 -25.791 29 -24.434 27	.326 5 .074 5 .107 4 .154 4	5.389 1. 5.597 1. 1.758 1.	.00 19.74 7 .00 23.50 6 .00 23.12 6 .00 25.07 8 .00 18.70 6	;
70	ATOM ATOM ATOM ATOM	566 N GLN 567 CA GLN	468 469 469 469	-25.675 28. -25.975 26. -27.174 26.	.881 7 .946 4 .745 3	.798 1. .534 1. .770 1.	00 23.45 16 00 24.47 7 00 24.99 6 00 27.22 6	

5	ATOM ATOM ATOM ATOM ATOM	570 CD GLN 571 OE1 GLN 572 NE2 GLN	469 469 469 469	-28.155 26.809 1.419 1.00 25.14 6 -27.857 26.844 -0.065 1.00 32.43 6 -26.710 26.700 -0.487 1.00 31.34 8 -28.896 27.052 -0.874 1.00 27.89 7
	ATOM ATOM ATOM ATOM	574 O GLN 575 N THR 576 CA THR	469 469 470 470	-27.901 25.483 4.266 1.00 27.60 6 -27.289 24.514 4.734 1.00 25.37 8 -29.206 25.548 4.115 1.00 28.73 7 -30.059 24.401 4.439 1.00 32.10 6
10	ATOM ATOM ATOM ATOM	578 OG1 THR 579 CG2 THR 580 C THR 581 O THR	470 470 470 470 470	-31.425 24.713 5.491 1.00 33.36 6 -30.619 25.555 6.553 1.00 45.26 8 -31.453 23.422 6.210 1.00 50.20 6 -30.737 23.976 3.138 1.00 32.77 6
15	ATOM ATOM ATOM ATOM	582 N GLY 583 CA GLY 584 C GLY 585 O GLY	471 471 471 471	-31.472 22.859 3.175 1.00 31.83 7 -32.224 22.397 2.033 1.00 27.97 6 -33.376 23.322 1.690 1.00 29.94 6
20	ATOM ATOM ATOM ATOM ATOM	586 N GLN 587 CA GLN 588 CB GLN 589 CG GLN 590 CD GLN	472 472 472 472 472	-33.842 24.159 2.594 1.00 24.86 7 -34.920 25.087 2.457 1.00 27.14 6 -35.868 24.892 3.667 1.00 27.31 6 -36.291 23.415 3.825 1.00 30.51 6
25	ATOM ATOM ATOM ATOM	591 OE1 GLN 592 NE2 GLN 593 C GLN 594 O GLN	472 472 472 472 472	-36.961 22.871 2.567 1.00 30.53 6 -37.981 23.425 2.161 1.00 39.95 8 -36.402 21.852 1.944 1.00 31.16 7 -34.530 26.561 2.441 1.00 29.60 6
30	ATOM ATOM ATOM ATOM ATOM	595 N THR 596 CA THR 597 CB THR 598 OG1 THR 599 CG2 THR	473 473 473 473	-33.248 26.912 2.380 1.00 25.83 7 -32.861 28.317 2.426 1.00 26.62 6 -32.278 28.731 3.792 1.00 26.64 6 -31.226 27.815 4.138 1.00 27.54
35	ATOM ATOM ATOM ATOM	599 CG2 THR 600 C THR 601 O THR 602 N SER 603 CA SER	473 473 473 474 474	-33.313 28.742 4.897 1.00 28.16 6 -31.824 28.643 1.371 1.00 26.31 6 -31.210 27.756 0.776 1.00 28.00 8 -31.685 29.939 1.074 1.00 28.62 7
4.0	ATOM ATOM ATOM ATOM	604 CB SER 605 OG SER 606 C SER 607 O SER	474 474 474 474	-30.592 30.261 0.112 1.00 29.44 6 -31.020 31.396 -0.803 1.00 30.45 6 -31.407 32.467 0.034 1.00 41.05 8 -29.366 30.471 0.992 1.00 26.65 6 -29.461 30.428 2 228 1.00 25.52 6
40	ATOM MOTA ATOM ATOM	608 N LEU 609 CA LEU 610 CB LEU 611 CG LEU	475 475 475 475	-28.178 30.585 0.442 1.00 29.47 7 -26.915 30.703 1.158 1.00 25.10 6 -25.749 30.725 0.159 1.00 27.83 6
45	ATOM ATOM ATOM	615 O LEU	475 475 475 475	-23.888 29.312 1.094 1.00 24.13 6 -23.349 31.446 -0.133 1.00 24.42 6 -26.884 31.893 2.087 1.00 25.84 6
50	ATOM ATOM ATOM ATOM ATOM	617 CA SER 618 CB SER 619 OG SER	476 476 476 476 476	-26.376 31.708 3.315 1.00 23.31 7 -26.357 32.857 4.219 1.00 25.20 6 -25.916 32.464 5.644 1.00 26.64 6 -24.514 32.203 5.624 1.00 29.43 8
55	ATOM ATOM ATOM ATOM ATOM	621 O SER 6 622 N ASP 6 623 CA ASP 6 624 CB ASP 6	476 177 177 177	-24.431 33.562 3.006 1.00 21.02 8 -25.506 35.127 4.241 1.00 22.24 7 -24.493 36.154 4.094 1.00 26.03 6 -24.907 37.504 4.683 1.00 20.27 6
60	ATOM ATOM ATOM ATOM ATOM	626 OD1 ASP 4 627 OD2 ASP 4 628 C ASP 4 629 O ASP 4	177 177 177 77	-25.914 38.190 3.758 1.00 25.73 6 -25.821 37.973 2.541 1.00 23.79 8 -26.769 38.912 4.292 1.00 28.92 8 -23.267 35.675 4.929 1.00 25.85 6 -23.423 34.962 5.914 1.00 24.00 8
65	ATOM ATOM ATOM ATOM	631 CD PRO 4 632 CA PRO 4 633 CB PRO 4 634 CG PRO 4	78 78 78 78 78	-22.998 36.108 4.492 1.00 27.37 7 -21.917 36.949 3.275 1.00 26.84 6 -20.849 35.736 5.098 1.00 25.42 6 -19.795 36.274 4.141 1.00 28.38 6
70	ATOM ATOM ATOM ATOM ATOM	635 C PRO 4 636 O PRO 4 637 N VAL 4	78 78 79 79	-20.453 37.280 3.272 1.00 27.24 6 -20.575 36.310 6.479 1.00 25.28 6 -21.006 37.407 6.820 1.00 23.68 8 -19.833 35.535 7.265 1.00 20.24 7 -19.287 36.005 8.535 1.00 18.86 6 -19.850 35.350 9.783 1.00 19.49 6

	ATOM ATOM ATOM	641 CG2 VA 642 C VA	L 479 L 479	-21.275 -17.777	35.907 1	0.036 1.	00 22.25 00 21.95 00 19.76	6 6 6
5	MOTA MOTA MOTA MOTA	643 O VAI 644 N HIS 645 CA HIS 646 CB HIS	5 480 5 480 5 480	-17.024 -15.584 -15.130	36.911 36.890	8.566 1. 8.387 1.	00 22.34 00 19.43 00 18.11 00 26.87	8 7 6 6
10	MOTA MOTA MOTA MOTA	647 CG HIS 648 CD2 HIS 649 ND1 HIS 650 CE1 HIS	480 480	-13.194 -12.637	38.112 37.883 38.169	7.293 1. 6.069 1. 8.176 1.	00 31.93 00 27.05 00 34.35 00 34.80	6 6 7 6
15	MOTA MOTA MOTA	651 NE2 HIS 652 C HIS 653 O HIS 654 N LEU	480 480	-11.831 -14.865 -15.096	37.850 6 36.679 9 37.370 10	6.210 1.6 9.718 1.6 9.709 1.6	00 34.81 00 23.08 00 23.37 00 19.18	7 6 8 7
	ATOM ATOM ATOM ATOM	655 CA LEU 656 CB LEU 657 CG LEU 658 CD1 LEU	481 481	-13.244 -13.567 -12.847	35.388 10 33.929 11 33.485 12	0.957 1.6 1.331 1.6 2.605 1.6	00 21.58 00 18.20 00 18.21	6 6 6
20	ATOM ATOM ATOM ATOM	659 CD2 LEU 660 C LEU 661 O LEU 662 N THR	481 481 481	-12.865 3 -11.747 3 -11.225 3	31.954 12 35.611 10 35.323 9	1.696 1.0 1.783 1.0 1.720 1.0	00 19.39 00 14.76 00 19.36 00 20.96	6 6 8
25	ATOM ATOM ATOM ATOM	663 CA THR 664 CB THR 665 OG1 THR	482 482 482	-9.642 3 -9.316 3 -9.907 3	86.403 11 87.916 11 88.515 10	.680 1.0	0 19.61 0 18.45 0 25.98 0 18.89	7 6 6 8
30	ATOM ATOM ATOM ATOM	667 C THR 668 O THR 669 N VAL	482 482 483	-8.971 3 -9.248 3 -8.075 3	5.766 12 6.131 14 4.821 12	.891 1.0 .035 1.0 .647 1.0	0 24.98 0 16.02 0 14.79 0 16.23	6 6 8 7
35	ATOM ATOM ATOM	671 CB VAL 672 CG1 VAL 673 CG2 VAL	483 483 483 483	-7.559 3 -7.051 3 -8.986 3	2.584 13 1.894 14 2.106 13	.530 1.0 .799 1.0	0 16.97 0 12.81 0 15.92 0 11.78	6 6 6
33	MOTA MOTA ATOM ATOM	674 C VAL 675 O VAL 676 N LEU 677 CA LEU	483 483 484 484	-5.261 3 -5.686 3	4.537 12. 5.110 15.	.918 1.00	0 19.97 0 18.57 0 16.89 0 19.89	6 8 7 6
40	ATOM ATOM ATOM ATOM	678 CB LEU 679 CG LEU 680 CD1 LEU 681 CD2 LEU	484 484 484 484	-4.621 3 -5.491 31 -5.927 39	7.080 15. 8.003 15. 9.176 15.	.890 1.00 .021 1.00 .868 1.00	18.15 23.40 25.20 20.46	6 6 6
45	ATOM ATOM ATOM ATOM	682 C LEU 683 O LEU 684 N PHE 685 CA PHE	484 484 485 485	-3.487 34 -3.928 33 -2.189 35	1.850 16. 3.975 16. 5.116 16.	228 1.00 975 1.00 218 1.00	22.29 23.90 21.03	6 8 7
50	ATOM ATOM ATOM ATOM	686 CB PHE 687 CG PHE 688 CD1 PHE 689 CD2 PHE	485 485 485	-0.399 33 0.440 32 -0.103 31	3.435 16. 2.516 17. .853 18.	333 1.00 184 1.00 266 1.00	22.92 21.76 27.90 28.30	6 6 6
	MOTA MOTA MOTA	690 CE1 PHE 691 CE2 PHE 692 CZ PHE	485 485 485 485	0.664 30 2.559 31		040 1.00 668 1.00	26.61 29.65 25.61 28.75	6 6 6
55	ATOM ATOM ATOM ATOM	693 C PHE 694 O PHE 695 N GLU 696 CA GLU	485 485 486 486	0.642 35 -1.023 35	.467 17. .866 17. .983 18. .104 19.	852 1.00 426 1.00 938 1.00	21.99 22.11 20.76 18.04	6 8 7 6
60	ATOM ATOM ATOM ATOM	697 CB GLU 698 CG GLU 699 CD GLU 700 OE1 GLU	486 486 486 486	-1.142 38 -0.711 39 -1.647 39	.403 19.3 .051 17.9 .818 17.0 .359 17.4	210 1.00 911 1.00 019 1.00	20.84 25.05 41.96	6 6 6
65	ATOM ATOM ATOM ATOM	701 OE2 GLU 702 C GLU 703 O GLU 704 N TRP	486 486 486 487	-1.429 39 -0.694 36 -1.588 36	.973 15.7 .840 21.1 .027 21.4	765 1.00 176 1.00 162 1.00	40.77 18.46 16.67	8 8 6 8
	ATOM ATOM ATOM ATOM	705 CA TRP 706 CB TRP 707 CG TRP	487 487 487	-0.328 37. 0.808 37. 1.922 36.	.235 23.5 .810 24.4 .843 24.6	153 1.00 111 1.00 187 1.00	13.01 18.40 21.87	7 6 6 6
70	ATOM ATOM ATOM	708 CD2 TRP 709 CE2 TRP 710 CE3 TRP	487 487 487	3.065 35.	690 25.5 061 25.5 128 26.2	21 1.00 26 1.00	21.14 24.31	6 6 6

5	MOTA MOTA MOTA MOTA MOTA MOTA	712 NE1 TRP 713 CZ2 TRP 714 CZ3 TRP 715 CH2 TRP	487 487 487 487 487	3.216 36.881 24.231 1.00 22.52 6 3.907 35.797 24.734 1.00 22.53 7 3.303 33.900 26.266 1.00 29.91 6 0.998 33.976 26.987 1.00 29.83 6 2.254 33.367 26.970 1.00 29.09 6 -1.599 37.899 24.068 1.00 15.44 6
10	ATOM ATOM ATOM ATOM ATOM ATOM	718 N LEU 719 CA LEU 720 CB LEU 721 CG LEU 722 CD1 LEU	488 488 488 488 488	-2.178 37.367 25.018 1.00 16.68 8 -2.036 38.993 23.447 1.00 14.44 7 -3.153 39.815 23.861 1.00 20.07 6 -2.596 40.924 24.783 1.00 17.49 6 -3.608 41.563 25.769 1.00 16.97 6 -4.062 40.567 26.830 1.00 17.38 6
15	ATOM ATOM ATOM ATOM ATOM	723 CD2 LEU 724 C LEU 725 O LEU 726 N VAL 727 CA VAL 728 CBA VAL	488 488 488 489 489	-2.987 42.813 26.370 1.00 13.93 6 -3.889 40.467 22.677 1.00 20.44 6 -3.255 41.009 21.752 1.00 19.65 8 -5.218 40.349 22.620 1.00 18.11 7 -5.998 40.940 21.542 1.00 14.66 6
20	ATOM ATOM ATOM ATOM ATOM	729 CBB VAL 730 CG1 VAL 731 CG1 VAL 732 CG2 VAL 733 CG2 VAL	489 489 489 489 489	-6.686 39.837 20.699 0.50 7.52 6 -6.677 39.925 20.604 0.50 13.86 6 -7.573 38.976 21.597 0.50 7.13 6 -5.696 39.457 19.543 0.50 15.87 6 -7.501 40.380 19.531 0.50 3.91 6
25	ATOM ATOM ATOM ATOM ATOM	734 C VAL 735 O VAL 736 N LEU 737 CA LEU	489 489 489 490	-7.264 38.776 21.402 0.50 18.65 6 -7.109 41.834 22.107 1.00 15.71 6 -7.689 41.604 23.179 1.00 14.52 8 -7.379 42.908 21.386 1.00 15.13 7 -8.520 43.733 21.703 1.00 13.72 6
30	ATOM ATOM ATOM ATOM ATOM	739 CG LEU 740 CD1 LEU 741 CD2 LEU 742 C LEU	490 490 490 490	-8.287 45.241 21.488 1.00 17.87 6 -9.650 45.888 21.873 1.00 26.07 6 -9.479 46.800 23.036 1.00 30.57 6 -10.373 46.403 20.662 1.00 25.07 6 -9.657 43.192 20.803 1.00 17.58 6
35	ATOM ATOM ATOM ATOM	743 O LEU 744 N GLN 745 CA GLN 746 CB GLN 747 CG GLN	490 491 491 491 491	-9.611 43.349 19.576 1.00 14.46 8 -10.673 42.568 21.412 1.00 15.83 7 -11.745 41.958 20.623 1.00 17.70 6 -12.252 40.628 21.264 1.00 15.03 6 -11.105 39.635 21.472 1.00 12.81 6
40	ATOM ATOM ATOM ATOM ATOM	748 CD GLN 749 OE1 GLN 750 NE2 GLN 751 C GLN 752 O GLN	491 491 491 491 491	-11.564 38.230 21.868 1.00 15.79 6 -12.023 38.043 22.988 1.00 14.61 8 -11.409 37.256 20.984 1.00 16.27 7 -12.971 42.824 20.375 1.00 17.71 6 -13.370 43.570 21.268 1.00 19.37 8
45	ATOM ATOM ATOM ATOM ATOM	753 N THR 754 CA THR 755 CB THR 756 OG1 THR 757 CG2 THR	492 492 492 492 492	-13.607 42.659 19.218 1.00 14.05 7 -14.853 43.378 18.934 1.00 19.01 6 -14.562 44.641 18.089 1.00 16.40 6 -15.769 45.381 17.905 1.00 18.39 8 -13.943 44.367 16.720 1.00 10.45 6
50	ATOM ATOM ATOM ATOM ATOM	758 C THR 759 O THR 760 N PRO 761 CD PRO 762 CA PRO	492 492 493 493 493	-15.803 42.450 18.173 1.00 18.96 6 -15.339 41.594 17.409 1.00 21.88 8 -17.095 42.713 18.251 1.00 18.78 7 -17.747 43.697 19.135 1.00 22.16 6
55	ATOM ATOM ATOM ATOM ATOM ATOM	763 CB PRO 764 CG PRO 765 C PRO 766 O PRO 767 N HIS 768 CA HIS	493 493 493 493 494	-19.352 42.063 18.371 1.00 24.99 6 -19.162 43.257 19.235 1.00 26.05 6 -18.285 42.504 16.138 1.00 27.02 6 -18.852 41.847 15.248 1.00 27.04 8 -17.978 43.797 15.960 1.00 24.22 7
60	ATOM ATOM ATOM ATOM ATOM	769 CB HIS 770 CG HIS 771 CD2 HIS 772 ND1 HIS	494 494 494 494	-18.114 44.445 14.651 1.00 25.72 6 -19.444 45.176 14.439 1.00 20.09 6 -20.639 44.279 14.595 1.00 21.67 6 -21.161 43.336 13.798 1.00 23.30 6 -21.380 44.271 15.754 1.00 27.49 7
65	ATOM ATOM ATOM ATOM ATOM	774 NE2 HIS 775 C HIS 776 O HIS 777 N LEU	494 494 494 495	-22.338 43.365 15.657 1.00 26.54 6 -22.211 42.788 14.482 1.00 32.10 7 -17.038 45.516 14.453 1.00 24.49 6 -16.481 46.028 15.429 1.00 24.01 8 -16.847 45.937 13.214 1.00 21.96 7
70	ATOM ATOM ATOM	779 CB LEU 780 CG LEU	495 495 495 495	-15.900 47.019 12.960 1.00 26.06 6 -15.014 46.748 11.741 1.00 26.66 6 -13.994 45.618 11.899 1.00 35.19 6 -13.449 45.265 10.525 1.00 25.66 6

	ATO ATO	M 783 C LEU	495 495	-12.895 45.958 12.900 1.00 24.13 6 -16.626 48.341 12.720 1.00 26.30 6
5	ATO	M 785 N GLU	495 496	-17.884 49.365 12.790 1.00 26.83 8
5	ATO: ATO:		496	-18.688 49.453 12.087 1.00 29.55
	ATO	1 788 CG GLU	496 496	-17.977 49.532 10.634 1.00 28.97 6
	ATON ATON		496	-18.414 49.757 8.168 1.00 42 07
10	ATOM		496 496	-19.560 50.157 7.882 1.00 41.53 8
	ATOM ATOM	792 C GLU	496	-19.995 49 201 12 205 1.00 45.31 8
	ATOM		496 497	-20.525 48.180 13.015 1.00 31.68 8
15	ATOM	795 CA PHE	497	-21.622 50 419 14.335 1.00 29.38 7
	ATOM ATOM		497 497	-21.388 50.515 15.832 1.00 29.88 6
	ATOM	798 CD1 PHE	497	-19.256 49.369 16.464 1.00 28.91 6
	MOTA MOTA		497 497	-21.311 48.363 17.131 1.00 27.06
20	MOTA	801 CE2 PHE	497	-20.622 47 321 17 710 1.00 23.29 6
	ATOM ATOM	802 CZ PHE 803 C PHE	497	-19.244 47.240 17.636 1.00 25.87 6
	ATOM	804 O PHE	497 497	22.433 31.633 13.861 1.00 31.11 6
25	MOTA MOTA	805 N GLN 806 CA GLN	498	-22.007 52.532 13.164 1.00 32.31 8 -23.726 51.653 14.219 1.00 34.14 7
	ATOM	806 CA GLN 807 CB GLN	498 498	-24.636 52.735 13.939 1.00 33.31 6
	ATOM ATOM	808 CG GLN 809 CD GLN	498	-26.207 51 444 12 256 1.00 38.13 6
20	ATOM	809 CD GLN 810 OE1 GLN	498 498	-25.763 52.154 11.097 1.00 49.99 6
30	MOTA MOTA	811 NE2 GLN	498	-24,603 51 778 10 563 1.00 32.38 8
	ATOM	812 C GLN 813 O GLN	498 498	-24.662 53.648 15.172 1.00 31.48 6
	ATOM	814 N GLU	499	-24.439 53.202 16.300 1.00 27.98 8 -24.990 54.911 14.000
35	ATOM ATOM	815 CA GLU 816 CB GLU	499 499	-25.112 55.888 16.009 1.00 32.56 6
	ATOM	817 CG GLU	499	-25.204 58 474 16 141 1.00 36.89 6
	ATOM ATOM	818 CD GLU 819 OE1 GLU	499 499	-24.771 59.578 15.184 1.00 48.45 6
40	MOTA	820 OE2 GLU	499	25.802 60.293 15.521 1.00 53.90 8
40	ATOM ATOM	821 C GLU 822 O GLU	499	-26.130 55.315 16.980 1.00 31.14 6
	ATOM	823 N GLY	499 500	-27.136 54.818 16.475 1.00 31.94 8
	ATOM ATOM	824 CA GLY	500	-26.874 54.743 19.217 1.00 32.19 7
45	ATOM	006	500 500	-26.643 53.325 19.696 1.00 31.51 6
	ATOM ATOM	827 N GLU	501	-25.948 52.497 18.921 1.00 30.30 8
	ATOM	000	501 501	-25.675 51.120 19.297 1.00 34.07 6
50	ATOM ATOM	830 CG GLU 5	01	-25,777 50 100 16 000 1.00 37.86 6
	ATOM		01 01	-24.984 49.346 15.895 1.00 49.17 6
	ATOM ATOM	833 OE2 GLU 5	01	-25,046 49 533 14 669 1.00 36.51 8
-	ATOM		01 01	-24.783 51.018 20.537 1.00 33.06 6
55	ATOM	836 N THR 5	02	-24.747 49.809 21 107 1 00 21 00 F
	ATOM ATOM		02 02	-23.870 49.563 22.248 1.00 32.85 6
	ATOM	839 OG1 THR 5	02	-25.546 49 428 24 021 1.00 35.75 6
60	ATOM ATOM		02	-23.532 48.289 24.441 1.00 35.82 6
	ATOM	842 O THR 5	02 02	-22.650 47 934 20.001 1.00 32.54 6
	ATOM ATOM	843 N ILE 50 844 CA ILE 50		-21.431 49.537 22.014 1.00 28 52 7
6 E	MOTA	845 CB ILE 50		-20.162 48.927 21.590 1.00 25.40 6
65	ATOM ATOM	846 CG2 ILE 50	3	-17.776 49.370 20.828 1.00 25.47
	ATOM	847 CG1 ILE 50 848 CD1 ILE 50		-19.669 50.786 19.971 1.00 21.79 6
	ATOM	849 C ILE 50	3 .	-19.624 48 113 22 767 1.00 19.73 6
70	ATOM ATOM	850 O ILE 50 851 N MET 50	3.	-19.439 48.685 23.853 1.00 23.06 8
	ATOM	852 CA MET 50		-19.443 46.807 22.591 1.00 24.90 7
				45.953 23.639 1.00 21.55 6

5	MOTA MOTA MOTA MOTA	854 CG MET 855 SD MET 856 CE MET	504 504	-19.797 44.769 23.963 1.00 33.48 6 -20.810 45.040 25.101 1.00 29.68 6 -21.940 43.610 25.242 1.00 46.02 16 -22.667 43.650 23.589 1.00 31.10 6
	ATOM ATOM ATOM ATOM ATOM	858 O MET 859 N LEU 860 CA LEU	504 505 505	-17.528 45.410 23.215 1.00 21.27 6 -17.374 44.875 22.106 1.00 22.96 8 -16.503 45.624 24.027 1.00 20.55 7 -15.134 45.198 23.728 1.00 22.33 6
10	MOTA MOTA MOTA MOTA MOTA	862 CG LEU 863 CD1 LEU 864 CD2 LEU 865 C LEU	505 505 505 505	-14.713 47.477 22.561 1.00 18.89 6 -13.796 48.688 22.489 1.00 19.44 6 -14.882 46.810 21.186 1.00 18.70 6 -14.567 44.307 24.817 1.00 20.15 6
15	MOTA MOTA ATOM MOTA	867 N ARG 868 CA ARG 869 CB ARG 870 CG ARG		-15.050 44.360 25.950 1.00 18.39 8 -13.523 43.542 24.483 1.00 18.25 7 -12.912 42.692 25.516 1.00 17.87 6 -13.607 41.313 25.508 1.00 14.96 6 -12.834 40.269 26.290 1.00 16.79 6
20	ATOM ATOM ATOM ATOM ATOM	871 CD ARG 872 NE ARG 873 CZ ARG 874 NH1 ARG 875 NH2 ARG	506 506 506 506 506	-13.699 39.078 26.757 1.00 19.51 6 -13.334 37.939 26.025 1.00 23.46 7 -12.990 36.692 26.065 1.00 24.43 6 -12.923 35.974 27.176 1.00 25.93 7
25	ATOM ATOM ATOM ATOM ATOM	876 C ARG 877 O ARG 878 N CYS 879 CA CYS 880 C CYS	506 506 507 507 507	-11.422 42.545 25.304 1.00 18.56 6 -10.998 42.387 24.142 1.00 20.43 8 -10.642 42.620 26.378 1.00 15.23 7 -9.189 42.447 26.292 1.00 14.89 6
30	ATOM ATOM ATOM ATOM	881 O CYS 882 CB CYS 883 SG CYS 884 N HIS	507 507 507 508	-8.934 40.975 26.583 1.00 15.28 6 -9.296 40.572 27.690 1.00 15.96 8 -8.438 43.301 27.322 1.00 14.55 6 -6.691 43.498 27.013 1.00 13.91 16 -8.446 40.213 25.604 1.00 15.07 7
35	ATOM ATOM ATOM ATOM ATOM	885 CA HIS 886 CB HIS 887 CG HIS 888 CD2 HIS 889 ND1 HIS	508 508 508 508 508	-8.334 38.763 25.811 1.00 11.91 6 -9.190 38.109 24.708 1.00 16.03 6 -9.119 36.626 24.572 1.00 16.94 6 -9.068 35.843 23.462 1.00 17.64 6
40	MOTA MOTA MOTA MOTA MOTA	890 CE1 HIS 891 NE2 HIS 892 C HIS 893 O HIS 894 N SER	508 508 508 508 509	-9.103 35.758 25.657 1.00 17.41 7 -9.034 34.516 25.215 1.00 17.37 6 -9.021 34.533 23.895 1.00 20.00 7 -6.925 38.219 25.733 1.00 11.83 6 -6.224 38.505 24.762 1.00 12.54 8 -6.515 37.364 26.654 1.00 13.70 7
45	ATOM ATOM ATOM ATOM ATOM	895 CA SER 896 CB SER 897 OG SER 898 C SER 899 O SER	509 509 509 509 509	-5.160 36.775 26.605 1.00 11.70 6 -4.583 36.732 28.041 1.00 13.47 6 -5.609 36.021 28.800 1.00 16.16 8 -5.190 35.407 25.970 1.00 14.21 6
50	ATOM ATOM ATOM ATOM ATOM	900 N TRP 901 CA TRP 902 CB TRP 903 CG TRP 904 CD2 TRP	510 510 510 510 510	-4.047 35.062 25.381 1.00 16.58 7 -3.860 33.764 24.708 1.00 16.04 6 -2.480 33.708 24.072 1.00 18.73 6 -2.187 32.441 23.306 1.00 21.24 6
55	ATOM ATOM ATOM ATOM ATOM ATOM	905 CE2 TRP 906 CE3 TRP 907 CD1 TRP 908 NE1 TRP 909 CZ2 TRP 910 CZ3 TRP	510 510 510 510 510 510	-1.193 30.505 22.616 1.00 25.92 6 -0.112 31.494 24.549 1.00 24.16 6 -2.827 31.958 22.214 1.00 22.22 6 -2.233 30.797 21.765 1.00 22.81 7 -0.276 29.462 22.568 1.00 24.18 6
60	ATOM ATOM ATOM ATOM ATOM	911 CH2 TRP 912 C TRP 913 O TRP 914 N LYS 915 CA LYS	510 510 510 511 511	0.698 29.433 23.526 1.00 31.04 6 -4.082 32.621 25.681 1.00 14.44 6 -3.665 32.647 26.852 1.00 17.08 8 -4.928 31.667 25.294 1.00 19.42 7
65	ATOM ATOM ATOM ATOM ATOM	916 CB LYS 917 CG LYS 918 CD LYS 919 CE LYS	511 511 511 511	-5.347 30.541 26.115 1.00 19.40 6 -4.131 29.625 26.418 1.00 21.00 6 -3.583 28.962 25.155 1.00 24.94 6 -2.124 28.579 25.337 1.00 34.17 6 -1.952 27.147 25.781 1.00 37.49 6
70	ATOM ATOM ATOM	921 C LYS 922 O LYS	511 511 511 512	-2.783 26.198 24.987 1.00 52.66 7 -5.940 30.945 27.450 1.00 20.33 6 -5.905 30.172 28.419 1.00 16.80 8 -6.444 32.171 27.602 1.00 18.28 7

	ATOM ATOM ATOM	925 CB AS	P 512	-6.989 32.633 28.861 1.00 20.31 6 -8.242 31.778 29.191 1.00 24.52 6
5	ATOM ATOM	927 OD1 AS	P 512	-9.306 32.129 28.155 1.00 31.39 6 -9.700 33.321 28.119 1.00 39.68 8
Ü	ATOM	929 C AS		-9.719 31.278 27.360 1.00 35.00 8 -6.015 32.663 30.018 1.00 23.40 6
	ATOM ATOM			-6.426 32.391 31.148 1.00 23.42 8
10	ATOM	932 CA LYS	5 513	-3.792 33.145 30.891 1.00 22 35 6
10	ATOM ATOM	933 CB LYS 934 CG LYS		-2.352 33.434 30.437 1.00 21.68 6
	ATOM ATOM	935 CD LYS 936 CE LYS	5 513	-0.232 32.292 29.608 1.00 28.34 6
1 5	ATOM	937 NZ LYS		0.269 31.086 28.816 1.00 32.92 6 0.196 29.791 29.554 1.00 33.55 7
15	MOTA MOTA	938 C LYS 939 O LYS		-4.352 34.269 31.748 1.00 19.86 6
	MOTA	940 N PRO	514	-4.890 35.263 31.264 1.00 21.45 8 -4.288 34.105 33.066 1.00 20.08 7
	MOTA MOTA	941 CD PRO 942 CA PRO		-3.701 32.938 33.768 1.00 16.95 6
20	ATOM ATOM	943 CB PRO	514	-4.548 34.574 35.342 1.00 19.22 6
	MOTA	944 CG PRO 945 C PRO		-4.169 33.133 35.176 1.00 21.34 6
	MOTA MOTA	946 O PRO 947 N LEU		-3.237 36.741 33.512 1.00 16.01 8
25	MOTA	948 CA LEU	515	-5.414 37.383 33.560 1.00 15.95 7 -5.081 38.762 33.215 1.00 17.10 6
	ATOM ATOM	949 CB LEU 950 CG LEU	515 515	-5.769 38.987 31.856 1.00 16.83 6
	ATOM	951 CD1 LEU	515	-5.790 40.368 31.231 1.00 21.64 6 -4.399 40.734 30.733 1.00 19.24 6
30	ATOM ATOM	952 CD2 LEU 953 C LEU	515 515	-6.777 40.380 30.043 1.00 19.80 6
	ATOM ATOM	954 O LEU	515	-6.788 39.666 34.569 1.00 18.84 R
	ATOM	956 CA VAL	516 516	-4.839 40.761 34.630 1.00 20.51 7
35	MOTA MOTA	957 CB VAL 958 CG1 VAL	516 516	-4.787 41.589 36.971 1.00 18.72 6
	ATOM	959 CG2 VAL	516	-5.313 40.319 37.644 1.00 22.67 6 -3.257 41.538 36.998 1.00 22.12 6
	ATOM ATOM	960 C VAL 961 O VAL	516 516	-4.807 43.163 35.073 1.00 19.73 6
40	MOTA	962 N LYS	517	-3.910 43.184 34.223 1.00 20.76 8 -5.268 44.251 35.693 1.00 17.34 7
40	ATOM ATOM	963 CA LYS 964 CB LYS	517 517	-4.760 45.576 35.381 1.00 20.33 6
	ATOM ATOM	965 CG LYS 966 CD LYS	517	-3.115 45.939 37.301 1.00 24.43 6
45	ATOM	967 CE LYS	517 517	-1.793 45.421 37.832 1.00 32.69 6 -0.798 46.552 38.056 1.00 40.27 6
40	ATOM ATOM	968 NZ LYS 969 C LYS	517 517	0.568 46.001 38.266 1.00 44.06 7
	MOTA	970 O LYS	517	-4.956 45.930 33.914 1.00 18.58 6 -4.026 46.331 33.234 1.00 24.35 8
. .	ATOM ATOM	971 N VAL 972 CA VAL	518 518	-6.181 45.803 33.417 1.00 20.45 7
50	ATOM ATOM	973 CB VAL 974 CG1 VAL	518	-7.756 45.223 31.607 1.00 12.17 6
	ATOM	975 CG2 VAL	518 518	-8.199 45.470 30.176 1.00 18.94 6 -7.408 43.737 31.794 1.00 16.75 6
	ATOM ATOM	976 C VAL 977 O VAL	518 518	-6.868 47.536 31.797 1.00 18.58 6
55	ATOM	978 N THR	519	-7.606 48.149 32.564 1.00 17.16 8 -6.307 48.063 30.711 1.00 15.94 7
	ATOM ATOM	979 CA THR 980 CB THR	519 519	-6.527 49.441 30.335 1.00 16.50 6
	ATOM	981 OG1 THR	519	-5.291 50.343 30.367 1.00 19.59 6 -4.770 50.456 31.693 1.00 23.11 8
60	ATOM ATOM	982 CG2 THR 983 C THR	519 519	-5.695 51.743 29.872 1.00 24.83 6
	ATOM ATOM	984 O THR	519	-6.436 48.736 28.095 1.00 14.36 8
	ATOM	985 N PHE 986 CA PHE	520 520	-8.121 50.187 28.643 1.00 14.86 7
65	MOTA MOTA	987 CB PHE 988 CG PHE	520 520	-10.122 50.069 27.240 1.00 15.51 6
	ATOM	989 CD1 PHE	520 520	-10.553 48.636 27.463 1.00 13.38 6 -10.748 48.165 28.750 1.00 20.15 6
	ATOM ATOM	990 CD2 PHE 991 CE1 PHE	520 520	-10.792 47.815 26.381 1.00 20.08 6
70	ATOM	992 CE2 PHE	520	-11.186 46.864 28.953 1.00 17.14 6 -11.230 46.499 26.578 1.00 22.12 6
, 0	ATOM ATOM	993 CZ PHE 994 C PHE	520 520	-11.423 46.048 27.867 1.00 17.10 6
				-8.279 51.650 26.721 1.00 17.13 6

5	ATON ATON ATON ATON ATON	996 N PHE 997 CA PHE 998 CB PHE 999 CG PHE 1 1000 CD1 PHE	521 521 521 521 521 521	-8.640 52.645 27.407 1.00 14.78 8 -7.626 51.700 25.575 1.00 16.20 7 -7.277 52.998 25.011 1.00 18.83 6 -5.799 53.045 24.616 1.00 13.50 6 -4.768 52.814 25.656 1.00 18.60 6 -4.368 51.527 26.017 1.00 17.37 6
10	MOTA MOTA MOTA MOTA MOTA MOTA	1 1002 CE1 PHE 1 1003 CE2 PHE 1 1004 CZ PHE 1 1005 C PHE 1 1006 O PHE	521 521 521 521 521 521	-4.208 53.905 26.334 1.00 18.44 6 -3.409 51.342 27.006 1.00 19.78 6 -3.260 53.693 27.313 1.00 22.69 6 -2.843 52.421 27.660 1.00 15.74 6 -8.074 53.327 23.749 1.00 18.44 6
15	ATOM ATOM ATOM ATOM	1008 CA GLN 1009 CB GLN 1010 CG GLN 1011 CD GLN	522 522 522 522 522 522	-8.333 54.613 23.480 1.00 19.35 7 -8.959 54.986 22.203 1.00 19.90 6 -10.396 55.487 22.317 1.00 16.32 6 -10.784 56.283 21.065 1.00 18.39 6
20	MOTA MOTA MOTA MOTA MOTA	1012 OE1 GLN 1013 NE2 GLN 1014 C GLN 1015 O GLN 1016 N ASN	522 522 522 522 523	-12.423 57.405 22.374 1.00 19.18 8 -12.700 57.470 20.153 1.00 24.51 7 -8.067 56.092 21.609 1.00 15.34 6 -7.789 57.034 22.321 1.00 17.30 8
25	ATOM ATOM ATOM ATOM ATOM	1017 CA ASN 1018 CB ASN 1019 CG ASN 1020 OD1 ASN 1021 ND2 ASN	523 523 523 523 523	-6.542 56.891 19.859 1.00 22.95 6 -7.241 58.158 19.332 1.00 19.57 6 -8.228 57.736 18.244 1.00 26.31 6 -8.013 56.813 17.441 1.00 19.76 8
30	ATOM ATOM ATOM ATOM ATOM	1022 C ASN 1023 O ASN 1024 N GLY 1025 CA GLY 1026 C GLY	523 523 524 524 524	-5.397 57.223 20.803 1.00 21.02 6 -4.911 58.341 20.918 1.00 19.19 8 -4.951 56.234 21.579 1.00 19.77 7 -3.852 56.350 22.495 1.00 16.41 6
35	ATOM ATOM ATOM ATOM ATOM	1027 O GLY 1028 N LYS 1029 CA LYS 1030 CB LYS 1031 CG LYS	524 525 525 525 525	-3.210 57.208 24.611 1.00 15.05 8 -5.405 57.256 24.133 1.00 13.81 7 -5.830 57.869 25.379 1.00 21.18 6 -6.700 59.128 25.247 1.00 14.85 6
40	ATOM ATOM ATOM ATOM ATOM	1032 CD LYS 1033 CE LYS 1034 NZ LYS 1035 C LYS 1036 O LYS	525 525 525 525 525 525	-7.406 61.279 26.281 1.00 22.51 6 -7.925 61.877 27.587 1.00 30.62 6 -8.822 63.048 27.330 1.00 36.72 7 -6.725 56.852 26.121 1.00 18.20 6
45	ATOM ATOM ATOM ATOM ATOM	1037 N SER 1038 CA SER 1039 CB SER 1040 OG SER 1041 C SER	526 526 526 526 526	-6.385 56.650 27.393 1.00 17.62 7 -7.107 55.625 28.155 1.00 20.03 6 -6.355 55.407 29.485 1.00 23.22 6 -7.317 55.093 30.466 1.00 38.12 8
50	ATOM ATOM ATOM ATOM ATOM	1042 O SER 1043 N GLN 1044 CA GLN 1045 CB GLN	526 527 527 527	-8.842 57.209 28.647 1.00 17.85 6 -9.490 55.148 28.254 1.00 17.16 7 -10.898 55.351 28.408 1.00 17.45 6 -11.723 54.793 27.225 1.00 20.82 6
55	ATOM ATOM ATOM ATOM	1047 CD GLN 1048 OE1 GLN 1049 NE2 GLN 1050 C GLN	527 527 527 527 527 527	-11.497 56.954 25.897 1.00 18.56 6 -12.606 57.450 26.116 1.00 31.62 8 -10.436 57.736 25.773 1.00 19.15 7 -11.386 54.615 29.661 1.00 20.94 6
60	ATOM ATOM ATOM ATOM	1052 N LYS 1053 CA LYS 1054 CB LYS 1055 CG LYS	528 528 528 528	-12.439 54.937 30.179 1.00 18.25 8 -10.643 53.581 30.032 1.00 21.18 7 -11.070 52.818 31.216 1.00 23.10 6 -12.177 51.832 30.842 1.00 21.83 6 -12.683 50.984 32.013 1.00 24.67 6
65	ATOM 1 ATOM 1 ATOM 1	1057 CE LYS 5 1058 NZ LYS 5 1059 C LYS 5 1060 O LYS 5	28 28 28 28	-13.739 49.961 31.589 1.00 18.23 6 -14.048 49.120 32.870 1.00 27.02 6 -15.081 48.072 32.574 1.00 24.24 7 -9.884 52.022 31.754 1.00 24.93 6
70	ATOM 1 ATOM 1 ATOM 1	1062 CA PHE 5 1063 CB PHE 5 1064 CG PHE 5	29 29 29 29 29	-9.678 52.044 33.062 1.00 20.79 8 -8.708 51.171 33.695 1.00 24.45 6 -7.610 51.940 34.458 1.00 25.50 6 -6.772 51.029 35.327 1.00 25.51 6 -5.799 50.236 34.762 1.00 19.40 6

5	ATON ATON ATON ATON ATON ATON	1 1067 CE 1 1068 CE 1 1069 CZ 1 1070 C 1 1071 O	1 PHE 5 22 PHE 5 PHE 5 PHE 5 PHE 5	529 -7. 529 -5. 529 -6. 529 -5. 529 -9. 529 -9.	026 49.375 249 50.078 262 49.292 480 50.289 388 50.817	36.700 35.535 37.491 36.902 34.687 35.359	1.00 29.98 1.00 25.00 1.00 28.84 1.00 32.29 1.00 27.88 1.00 30.99	6 6 6
10	MOTA ATOM ATOM MOTA MOTA	1073 CA 1074 CB 1075 OG 1076 C	SER 5 SER 5 SER 5 SER 5	30 -9.3 30 -9.3 30 -11.0 30 -11.2 30 -8.3	779 48.225 925 47.522 971 46.401 977 47.199	34.853 35.917 35.422 36.250 36.434	1.00 26.67 1.00 24.98 1.00 21.29 1.00 25.72 1.00 24.39	7 6 6 8 6
15	ATOM ATOM ATOM ATOM ATOM	1079 CA 1080 CB 1081 CG 1082 CD	HIS 5: HIS 5: HIS 5: HIS 5:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	168 46.977 10 45.965 04 45.948 59 47.160	35.576 37.730 38.204 39.737 40.197 40.642	1.00 24.91 1.00 22.12 1.00 23.65 1.00 28.35 1.00 23.57 1.00 18.55	8 7 6 6
20	MOTA MOTA ATOM ATOM ATOM ATOM ATOM ATOM	1084 CE1 1085 NE2 1086 C 1087 O	HIS 53 HIS 53 HIS 53 HIS 53	31 -5.4 31 -5.0 31 -6.1 41 -8.1 -7.2	78 47.200 95 48.388 73 49.102 08 44.552	40.170 40.617 40.890 37.814	1.00 26.69 1.00 16.65 1.00 23.94 1.00 23.89 1.00 26.21	6 7 6 7 6 8
25	ATOM ATOM ATOM ATOM ATOM		LEU 53 LEU 53 LEU 53 LEU 53 LEU 53 LEU 53	2 -9.89 2 -10.63 2 -10.03 2 -11.03	36 42.966 30 42.505 22 42.782 73 42.550	37.689 37.480 38.760 40.148	1.00 21.77 1.00 20.70 1.00 30.28 1.00 26.56 1.00 29.07	7 6 6 6
30	ATOM ATOM ATOM ATOM ATOM	1094 C 1095 O 1096 N 1097 CA 1098 CB	LEU 53 LEU 53 LEU 53 ASP 53 ASP 53 ASP 53	2 -10.76 2 -10.79 3 -11.54 3 -12.46	42.722 4 41.540 1 43.685 9 43.465	40.435 1 36.279 1 35.900 1 35.778 1 34.679 1	1.00 24.99 1.00 22.94 1.00 22.01 1.00 21.75	6 6 8 7 6
35	MOTA MOTA MOTA MOTA MOTA	1099 CG 1100 OD1	ASP 533 ASP 533 ASP 533 ASP 533	3 -14.73 3 -14.83 -15.59 -11.84	4 44.545 7 43.612 7 45.472 3 43.636	33.915 1 33.083 1 34.000 1 33.296 1	.00 29.71 .00 32.90 .00 32.91 .00 36.01 .00 25.88	6 8 8 6
40	ATOM ATOM ATOM ATOM ATOM	1104 N 1105 CD 1106 CA 1107 CB 1108 CG	PRO 534 PRO 534 PRO 534 PRO 534 PRO 534	-11.85 -12.34 -11.29 -10.889	7 42.605 3 7 41.246 3 8 42.681 3 9 41.204 3	32.460 1 32.778 1 11.112 1 0.870 1	.00 24.36 .00 24.65 .00 22.97 .00 24.00 .00 24.02	8 7 6 6
45	MOTA MOTA MOTA MOTA MOTA	1109 C 1110 O 1111 N 1112 CA	PRO 534 PRO 534 THR 535 THR 535 THR 535	-12.256 -11.970 -13.420 -14.424 -15.748	43.102 3 42.936 2 43.654 3 44.061 2	0.017 1. 8.824 1. 0.350 1. 9.401 1.	.00 23.04 .00 22.11 .00 19.00 .00 21.43	6 8 7 6
50	ATOM ATOM ATOM ATOM ATOM	1114 OG1 1 1115 CG2 1 1116 C 1 1117 O 1	THR 535 THR 535 THR 535 THR 535 THR 535 PHE 536	-16.331 -15.461 -14.747 -14.445 -15.267	43.801 3 41.797 2 45.554 2 46.237 3	0.796 1. 9.706 1. 9.451 1. 0.423 1.	00 27.24 00 24.99 00 26.07 00 23.58 00 26.14	6 8 6 6 8
55	ATOM ATOM ATOM ATOM ATOM	1119 CA I	PHE 536 PHE 536 PHE 536 PHE 536	-15.549 -14.343 -14.408 -14.528	47.475 28 48.160 27 49.616 27 50.596 28	3.150 1. 7.523 1. 7.170 1.	00 20.63 00 20.10 00 25.47 00 25.61 00 27.00	7 6 6 6 6
60	ATOM ATOM ATOM MOTA	1124 CE1 P 1125 CE2 P 1126 CZ P 1127 C P	HE 536	-14.332 -14.571 -14.385 -14.493 -16.796	51.937 27 51.350 25 52.317 26 47.669 27	.787 1.0 .490 1.0 .463 1.0 .297 1.0	00 32.62 00 28.46 00 30.41 00 24.00	6 6 6 6
65	ATOM ATOM ATOM ATOM	1129 N S 1130 CA S 1131 CB S 1132 OG S	ER 537 ER 537 ER 537 ER 537 ER 537	-16.952 -17.665 -18.914 -20.120 -20.769	48.572 27 48.856 27 48.448 27 47.307 27	.730 1.0 .050 1.0 .908 1.0 .412 1.0	00 24.50 00 21.97 00 26.52 00 30.03 00 44.19	3 7 5
70	ATOM :		ER 537 LE 538	-19.128 -18.911 -19.654 -20.004	51.172 27. 50.702 25.	.721 1.0 .686 1.0	0 27.38 6 0 27.33 8 0 25.86 7 0 29.46 6	5

5	NOTA NOTA NOTA NOTA NOTA NOTA	1138 1139 1140 1141 1142	CB ILE CG2 ILE CG1 ILE CD1 ILE C ILE O ILE N PRO	538 538	-19.1 -19.6 -17.6 -16.8 -21.4 -21.7	69 54.11 79 52.66 17 52.71 77 51.99 68 51.48	8 23.94 9 24.47 1 23.22 1 24.92 9 23.84	1 1.00 27.2 2 1.00 30.5 3 1.00 29.5 5 1.00 29.8 9 1.00 27.9	3 5 3 8 9
10	MOTA MOTA MOTA MOTA MOTA	1145 c 1146 c 1147 c 1148 c	CD PRO CA PRO CB PRO CG PRO C PRO	539 539 539 539 539	-22.03 -23.7 -24.38 -23.24	18 52.92 76 52.46 30 52.65 18 52.48	8 27.184 8 25.598 3 26.983 2 27.950	1.00 32.73 1.00 33.85 1.00 36.13 1.00 34.99	3 5 3 6
15	MOTA MOTA MOTA MOTA MOTA	1150 N 1151 C 1152 C		539 540 540 540 540	-23.32 -24.97 -25.28 -26.22 -27.51	24 54.70 74 53.65 8 54.75 3 55.742	6 24.888 3 23.827 6 22.935 2 23.631	1.00 38.22 1.00 36.97 1.00 35.17 1.00 43.87	? 6
20	MOTA MOTA MOTA MOTA MOTA	1155 o		540 540 540 540 540	-27.88 -28.14 -27.88 -24.06 -23.67	3 55.584 5 56.782 3 54.705 0 55.448	25.468 25.593 26.468 22.362	1.00 49.77 1.00 56.21 1.00 57.44 1.00 57.25 1.00 34.61	6 8 7 6
25	ATOM ATOM ATOM ATOM ATOM	1159 N 1160 C 1161 C 1162 C 1163 O	ALA ALA A	541 541 541 541 541	-23.47 -22.28 -21.77 -22.56	3 54.755 7 55.232 8 54.121 1 56.466	21.391 20.694 19.774 19.832	1.00 33.34 1.00 29.80 1.00 30.02 1.00 27.89 1.00 29.52	8 7 6 6
30	ATOM ATOM ATOM ATOM ATOM	1164 N 1165 CA 1166 CE 1167 CG	ASN A ASN B ASN	542 542 542 542	-23.650 -21.520 -21.642 -21.985 -21.012	57.284 58.431 59.727 60.117		1.00 29.60 1.00 30.60 1.00 31.55 1.00 30.39 1.00 31.63	8 7 6 6 6
35	ATOM ATOM ATOM ATOM ATOM	1169 NE 1170 C 1171 O 1172 N	2 ASN ASN ASN HIS	542 542 542 542 543	-19.838 -21.479 -20.357 -19.453 -20.223	60.127 58.545 57.698 59.609	20.268 21.781 17.936 18.122 17.134	1.00 27.57 1.00 33.23 1.00 32.33 1.00 29.09 1.00 29.40	8 7 6 8 7
40	ATOM ATOM ATOM ATOM	1177 ND	HIS	543 543 543 543 543	-19.075 -19.262 -20.360 -20.704 -21.278	60.971 60.632	16.266 15.272 14.295 13.740 13.822	1.00 28.82 1.00 24.51 1.00 31.72 1.00 33.88 1.00 32.86	6 6 6
45	ATOM ATOM ATOM ATOM MOTA		1 HIS 2 HIS HIS HIS SER	543 543 543 543 544	-22.117 -21.794 -17.747 -16.696 -17.812	60.939 59.664 60.009 59.768	13.008 12.941 16.976 16.366	1.00 31.84 1.00 31.48 1.00 26.62 1.00 25.96	7 6 7 6 8
50	MOTA MOTA MOTA MOTA MOTA	1183 CA 1184 CB 1185 OG 1186 C 1187 O	SER SER SER SER	544 544 544 544	-16.557 -16.839 -17.739 -15.976	60.454 60.738 61.887 61.477 59.443	18.221 18.941 19.915 20.930 19.474	1.00 20.85 1.00 24.82 1.00 30.28 1.00 39.11 1.00 24.89	7 6 6 8 6
55	ATOM ATOM ATOM ATOM ATOM	1188 N 1189 CA 1190 CB 1191 CG 1192 CD2	HIS HIS HIS	544 545 545 545 545 545	-14.775 -16.746 -16.306 -17.474 -18.145 -17.620	59.348 58.344 57.005 56.104 56.654 56.980	19.463 19.811 20.302 21.534	1.00 25.22 1.00 20.33 1.00 19.38 1.00 19.40 1.00 18.37	8 7 6 6
60	ATOM ATOM ATOM ATOM ATOM	1193 ND1 1194 CE1 1195 NE2 1196 C 1197 O	HIS HIS HIS HIS	545 545 545 545 545	-19.493 -19.768 -18.643 -15.589 -15.013	56.901 57.374 57.454 56.313	21.627 22.829 23.525 18.657	1.00 18.22 1.00 23.55 1.00 26.33 1.00 21.05 1.00 22.05 1.00 21.86	6 7 6 7 6
65	ATOM ATOM	1198 N 1199 CA 1200 CB 1201 OG 1202 C	SER SER SER SER SER SER	546 546 546 546	-15.569 -14.833 -15.075 -16.442 -13.339	56.869 56.217 56.857 56.712	17.440 1 16.363 1 14.986 1 14.613 1	1.00 20.66 1.00 19.96 1.00 20.48 1.00 25.61	8 7 6 8
70	MOTA MOTA	1206 C	SER 5 GLY 5 GLY 5 GLY 5	546 547 547 547	-12.915 -12.556 -11.123 -10.385	57.252 55.288 55.483 54.152	17.287 1 16.197 1 16.411 1 16.555 1	.00 20.51 .00 22.06 .00 16.70 .00 20.49 .00 22.63 .00 16.09	6 7 6 6 8

	ATOM ATOM ATOM	1209	N AS CA AS CB AS	P 548	-9.11 -8.32	4 53.08	9 17.121	1.00 21.5	7 6
-	ATOM		CG AS		-6.88 -6.81				-
5	MOTA MOTA		OD1 AS		-7.84	9 53.52	8 14.540		
	MOTA		OD2 AS:		-5.76 -8.31				
	ATOM	1215	O AS	P 548	-7.81				-
10	ATOM ATOM		N TY		-8.82	2 51.420	6 18.798	1.00 16.97	7
	ATOM		CB TY		-8.81 -10.19				-
	ATOM ATOM		CG TY		-11.27	2 51.332			
	ATOM	1220 1221	CD1 TYP		-11.90 -12.87				6
15	ATOM	1222	CD2 TYP	549	-11.67				
	MOTA MOTA	1223 1224	CE2 TYP		-12.63		22.116	1.00 15.60	6
	ATOM	1225	OH TYP		-13.23 -14.21			1.00 18.77 1.00 18.41	
20	ATOM ATOM	1226	C TYP		-7.76	7 49.805	20.355	1.00 15.78	8 6
20	ATOM	1227 1228	O TYP N HIS		-7.539 -7.19			1.00 15.86	8
	MOTA	1229	CA HIS	550	-6.24			1.00 15.01 1.00 12.99	7 6
	MOTA MOTA	1230 1231	CB HIS		-4.849		21.372	1.00 11.96	6
25	ATOM	1232	CD2 HIS		-3.942 -2.944			1.00 17.71 1.00 16.09	6 6
	ATOM ATOM	1233 1234	ND1 HIS	550	-3.988	51.206	21.971	1.00 11.60	7
	ATOM	1235	CE1 HIS NE2 HIS	550 550	-3.058 -2.407			1.00 16.95	6
30	ATOM	1236	C HIS	550	-6.263	48.596		1.00 19.22 1.00 13.37	7 6
30	ATOM ATOM	1237 1238	O HIS N CYS	550 551	-6.922 -5.680		24.129	1.00 12.78	8
	MOTA	1239	CA CYS	551	-5.670		23.957 25.414	1.00 14.21 1.00 15.38	7 6
	MOTA MOTA	1240 1241	C CYS	551 551	-4.301		25.880	1.00 16.27	6
35	ATOM	1242	CB CYS	551 551	-3.422 -6.746	46.462 46.304	25.132 25.856	1.00 15.15 1.00 16.85	8
	ATOM ATOM	1243	SG CYS	551	-6.581	44.597	25.248	1.00 14.82	6 16
	ATOM	1244 1245	N THR	552 552	-4.080 -2.875	47.061	27.186	1.00 17.41	7
40	ATOM	1246	CB THR	552	-1.899	46.643 47.735	27.862 28.305	1.00 17.27 1.00 21.80	6 6
40	ATOM ATOM		OG1 THR	552 552	-2.527	48.654	29.205	1.00 17.53	8
	ATOM		C THR	552 552	-1.356 -3.346	48.478 45.877	27.075 29.127	1.00 17.12 1.00 19.83	6
	ATOM ATOM		O THR	552	-4.471	46.142	29.600	1.00 16.21	6 8
45	ATOM		N GLY CA GLY	553 553	-2.496 -2.815	44.953 44.160	29.534 30.731	1.00 17.84	7
	MOTA		C GLY	553	-1.647	43.261	31.108	1.00 20.33 1.00 18.60	6 6
	ATOM ATOM		O GLY N ASN	553 554	-0.779 -1.603	42.951	30.293	1.00 19.87	8
ΕΛ	ATOM	1256	CA ASN	554	-0.560	42.866 42.051	32.373 32.959	1.00 20.99 1.00 20.36	7 6
50	ATOM ATOM		CB ASN	554	-0.512	42.310	34.478	1.00 26.77	6
	ATOM		DD1 ASN	554 554	0.800 1.700	42.938 42.286	34.897 35.441	1.00 40.91	6
	ATOM ATOM		VD2 ASN	554	0.927	44.227	34.633	1.00 46.67	8 7
55	ATOM	1261 (1262 (554 554	-0.879 -1.973	40.566 40.181		1.00 22.51	6
	ATOM	1263 N	ILE	555	0.018	39.799		1.00 22.15 1.00 19.40	8 7
	ATOM ATOM		A ILE	555 555	-0.198	38.352	32.139	1.00 22.27	6
<i>C</i> 0	ATOM	1266 C	G2 ILE	555	-0.210 -0.327	37.750 36.226		1.00 26.29 1.00 23.31	6 6
60	ATOM ATOM		G1 ILE	555	-1.367	38.322		1.00 28.16	6
	ATOM	1269 C	D1 ILE ILE	555 55 5	-1.371 0.974	37.992 37.777		1.00 29.42	6
	ATOM	1270 o	ILE	555	2.112	38.140		1.00 27.67 1.00 24.10	6 8
65	ATOM ATOM	1271 N 1272 C		556 556	0.732	37.028	34.020	1.00 33.10	7
	ATOM	1273 C	GLY	556	1.942 2.447	36.581 37.813		1.00 37.62 1.00 38.80	6 6
	MOTA MOTA	1274 O 1275 N	-	556 557	1.659	38.354	36.299	1.00 43.91	8
7.0	MOTA	1276 C		557 557	3.655 4.182			1.00 41.47 1.00 43.65	7
70	ATOM ATOM	1277 CI	B TYR	557	5.381	39.224	36.832 1	1.00 43.65	6 6
	AION	1278 C	3 TYR	557	5.020	38.274	37.961 1	1.00 57.42	6

5	MOTA MOTA MOTA MOTA MOTA MOTA	4 128 4 128 4 128 4 128 4 128 4 128	10 C 11 C 12 C 13 C 14 O 15 C	H TYR	8 557 8 557 8 557 8 557 8 557 8 557	5.52 5.1 4.14 3.78 4.31 3.97 4.67	79 36.10 40 38.66 38 37.78 13 36.51 79 35.62	38.99 38.96 38.96 7 39.98 3 39.98 9 40.98	2 1.00 62.5 3 1.00 61.00 2 1.00 63.0 6 1.00 63.5 4 1.00 66.68	7 6 0 6 3 6 6 6 8 8
10	ATOM ATOM ATOM ATOM ATOM ATOM	1 128 1 128 1 128 1 129	7 N 8 C2 9 CE 0 OG	THR	558 558 558 558	5.44 4.29 4.72 5.26 6.23	98 40.31 2 41.17 60 40.26 7 39.39	6 35.115 9 33.594 3 32.496 9 31.364 5 31.942	5 1.00 41.33 4 1.00 36.77 5 1.00 30.71 4 1.00 30.82	8 8 7 7 1 6 1 6
15	MOTA MOTA MOTA MOTA	129 129 129 129	2 C 3 O 4 N 5 CA	-	558 558 559 559	5.85 3.53 2.52 3.68 2.61	2 41.92 1 41.25 9 43.20 7 43.94	2 31.912 7 31.642 2 31.609 2 30.960	1.00 25.66 1.00 24.50 1.00 21.00	6 6 8 7
20	ATOM ATOM ATOM ATOM ATOM	129 1298 1298 1300	7 CG 8 CD 9 CD 0 C	LEU LEU LEU LEU	559 559 559 559 559	2.73 1.60 0.32 1.97 2.65	1 46.379 3 46.049 9 47.830	30.958 31.713 31.316	1.00 26.53 1.00 27.15 1.00 25.15 1.00 28.75	
25	MOTA MOTA MOTA MOTA	1301 1302 1303 1304 1305	N CA CB CG	PHE	559 560 560 560 560	3.71: 1.484 1.430 0.82: 1.848	43.470 43.290 41.920	28.844 28.855 27.409 27.060		8 7 6 6
30	ATOM ATOM ATOM ATOM ATOM	1306 1307 1308 1309 1310	CD: CE:	PHE PHE PHE PHE	560 560 560 560 560	1.971 2.645 2.903 3.582 3.704	40.190 40.457 39.157 39.445	28.442 26.156 28.588	1.00 24.86 1.00 21.03 1.00 29.44 1.00 19.89	6 6 6
35	ATOM ATOM ATOM ATOM ATOM	1311 1312 1313 1314 1315	0	PHE PHE SER SER SER	560 560 561 561 561	0.521 -0.346 0.753 -0.087 0.744	44.353 44.884 44.626 45.564	26.794 27.504 25.521 24.785	1.00 25.34 1.00 17.36 1.00 18.36 1.00 17.60 1.00 14.63	6 8 7 6
40	MOTA MOTA ATOM MOTA MOTA	1316 1317 1318 1319 1320	OG C O N CA	SER SER SER SER SER	561 561 561 562 562	-0.115 -0.662 0.101 -1.921	47.812 44.829 44.113 45.070	24.188 23.901 23.561 22.894 23.232	1.00 20.14 1.00 21.55 1.00 18.96 1.00 19.79 1.00 16.19	6 8 6 8 7
45	ATOM ATOM ATOM ATOM ATOM	1321 1322 1323 1324	CB OG C O	SER SER SER SER	562 562 562 562	-2.518 -4.029 -4.801 -2.322 -1.949	44.462 44.188 45.336 45.381 46.561	22.049 22.233 21.900 20.845 20.987	1.00 16.74 1.00 16.78 1.00 21.00 1.00 18.24 1.00 16.85	6 8 6 8
50	ATOM ATOM ATOM ATOM	1325 1326 1327 1328 1329	N CA CB CG CD	LYS LYS LYS LYS LYS	563 563 563 563 563	-2.535 -2.484 -2.369 -1.228 0.128	44.839 45.663 44.909 43.981 44.595	19.652 18.445 17.133 16.902 16.685	1.00 17.96 1.00 17.36 1.00 20.94 1.00 25.34 1.00 29.02	7 6 6 6 6
55	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1330 1331 1332 1333 1334 1335	CE NZ C O N CD	LYS LYS LYS LYS PRO PRO	563 563 563 563 564 564	0.954 0.495 -3.821 -4.817 -3.840 -2.702	43.735 42.308 46.400 45.960 47.518 48.123	15.721 15.692 18.391 18.978 17.696 16.952	1.00 42.35 1.00 38.14 1.00 17.27 1.00 16.54 1.00 18.39 1.00 20.79	6 7 6 8 7
60	ATOM ATOM ATOM ATOM ATOM	1336 1337 1338 1339 1340	С	PRO PRO PRO PRO PRO	564 564 564 564	-5.060 -4.545 -3.254 -6.032	48.294 49.689 49.450 47.697	17.546 17.142 16.475 16.528	1.00 19.84 1.00 17.33 1.00 21.76 1.00 19.62	6 6 6
65	MOTA MOTA MOTA MOTA	1341 1342 1343 1344	N CA CB CG1	VAL VAL VAL	564 565 565 565 565	-5.723 -7.295 -8.427 -9.405 -10.418	46.924 48.033 47.704 46.676 46.223	16.674 15.841 16.450	1.00 19.46 1.00 17.22 1.00 20.36 1.00 20.84 1.00 20.46	8 7 6 6
70	ATOM ATOM ATOM ATOM MOTA	1345 1346 1347 1348 1349	O Y	VAL VAL THR	565 565 565 566 566	-8.699 -9.173 -9.532 -9.444 -10.111	45.391 49.033 49.772 49.317	16.899 15.590 16.499 14.320	1.00 23.72 1.00 22.05 1.00 22.10 1.00 24.93 1.00 26.07	6 6 8 7 6

5	MOTA MOTA MOTA MOTA MOTA	1351 OG1 THE 1352 CG2 THE 1353 C THE	566 566 566 566	-9.631 51.082 12.579 1.00 31.66 6 -9.737 50.055 11.569 1.00 38.39 8 -8.180 51.513 12.694 1.00 23.71 6 -11.611 50.269 13.909 1.00 25.06 6 -11.985 49.330 13.244 1.00 21.88 8
10	ATOM ATOM ATOM ATOM ATOM ATOM	1356 CA ILE 1357 CB ILE 1358 CG2 ILE 1359 CG1 ILE 1360 CD1 ILE 1361 C ILE	567 567 567	-12.362 50.988 14.714 1.00 21.40 7 -13.784 50.959 14.909 1.00 25.06 6 -14.088 50.702 16.424 1.00 26.21 6 -15.588 50.707 16.673 1.00 26.68 6 -13.415 49.394 16.825 1.00 26.56 6 -13.946 48.548 17.939 1.00 30.83 6 -14.416 52.294 14.501 1.00 24.36 6
15	MOTA MOTA ATOM ATOM ATOM AOTA MOTA	1362 O ILE 1363 N THR 1364 CA THR 1365 CB THR 1366 OG1 THR	567 568 568 568 568	-14.013 53.384 14.920 1.00 23.36 8 -15.412 52.275 13.630 1.00 22.83 7 -16.083 53.461 13.152 1.00 27.27 6 -15.945 53.600 11.622 1.00 31.88 6 -14.565 53.495 11.277 1.00 32.11 8
20	ATOM ATOM ATOM ATOM ATOM	1367 CG2 THR 1368 C THR 1369 O THR 1370 N VAL 1371 CA VAL	568 568 569 569	-16.462 54.972 11.179 1.00 34.54 6 -17.575 53.452 13.501 1.00 28.53 6 -18.190 52.383 13.508 1.00 32.64 8 -18.090 54.606 13.863 1.00 23.55 7 -19.472 54.855 14.163 1.00 27.27 6
25	ATOM ATOM ATOM ATOM ATOM	1372 CB VAL 1373 CG1 VAL 1374 CG2 VAL 1375 C VAL 1376 O VAL	569 569 569 569	-19.728 55.507 15.523 1.00 28.51 6 -21.227 55.733 15.757 1.00 26.42 6 -19.189 54.706 16.696 1.00 27.97 6 -20.011 55.844 13.098 1.00 32.65 6 -19.332 56.810 12.710 1.00 33.21 8
30	ATOM MOTA ATOM ATOM MOTA	1377 N GLN 1378 CA GLN 1379 CB GLN 1380 CG GLN 1381 CD GLN	570 570 570 570 570	-21.245 55.670 12.689 0.01 33.85 7 -21.966 56.476 11.737 0.01 35.75 6 -23.335 56.839 12.362 0.01 36.48 6 -24.465 56.854 11.347 0.01 37.54 6 -25.478 55.756 11.599 0.01 37.91 6
35	ATOM ATOM ATOM ATOM	1382 OE1 GLN 1383 NE2 GLN 1384 C GLN 1385 O GLN 1386 N VAL	570 570 570 570 571	-25.142 54.680 12.096 0.01 38.17 8 -26.735 56.020 11.257 0.01 38.21 7 -21.355 57.778 11.241 0.01 36.70 6 -21.049 58.699 11.995 0.01 36.81 8 -21.273 57.907 9.919 0.01 37.51 7
40	ATOM ATOM ATOM ATOM ATOM	1387 CA VAL 1388 CB VAL 1389 CG1 VAL 1390 CG2 VAL 1391 C VAL	571 571 571 571 571	-20.781 59.094 9.240 0.01 38.20 6 -19.483 59.658 9.842 0.01 38.61 6 -18.334 58.667 9.681 0.01 38.88 6 -19.115 60.985 9.180 0.01 38.83 6
45	ATOM ATOM ATOM ATOM ATOM	1392 O VAL 1 OWO WAT 2 OWO WAT 3 OWO WAT 4 OWO WAT	571 601 602 603 604	-21.420 59.293 6.949 0.01 38.53 8 -13.958 32.760 19.930 1.00 18.36 8 -13.653 59.625 23.320 1.00 24.59 8 -5.895 43.456 18.965 1.00 14.14 8
50	ATOM ATOM ATOM ATOM ATOM	5 OWO WAT 6 OWO WAT 7 OWO WAT 8 OWO WAT 9 OWO WAT	605 606 607 608 609	-8.700 36.412 28.355 1.00 21.65 8 -25.548 35.202 7.898 1.00 24.88 8 -2.902 48.395 31.897 1.00 19.13 8 -14.303 55.610 23.676 1.00 24.28 8
55	ATOM ATOM ATOM ATOM ATOM	10 OW0 WAT 11 OW0 WAT 12 OW0 WAT 13 OW0 WAT 14 OW0 WAT	610 611 612 613 614	-12.433 34.237 21.505 1.00 14.04 8 -5.417 53.367 21.002 1.00 16.89 8 -29.599 18.069 11.595 1.00 34.62 8 -17.813 30.679 2.648 1.00 16.34 8
60	ATOM ATOM ATOM ATOM ATOM	16 OWO WAT 17 OWO WAT 18 OWO WAT 19 OWO WAT	615 616 617 618 619	-21.191 20.720 5.335 1.00 30.05 8 -15.621 34.100 18.319 1.00 18.82 8 -6.528 44.456 14.460 1.00 26.68 8 -6.213 31.143 22.792 1.00 19.89 8
65	ATOM ATOM ATOM ATOM ATOM	20 OWO WAT 21 OWO WAT 22 OWO WAT 23 OWO WAT	620 621 622 623 524	2.277 38.630 20.953 1.00 28.34 8 -20.151 29.522 0.183 1.00 21.62 8 -27.773 35.663 6.295 1.00 20.74 8 0.481 42.002 19.811 1.00 24.67 8
70	ATOM ATOM ATOM ATOM	25 OWO WAT 6 26 OWO WAT 6	525 526	-17.815 32.952 1.120 1.00 26.99 8 -16.604 36.105 25.523 1.00 18.45 8 0.330 41.286 22.516 1.00 29.01 8 -13.324 59.911 17.129 1.00 40.98 8 -9.214 59.486 22.450 1.00 41.91 8

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	ATOM	29	OMO MAN	620	00 144				
	ATOM	30	OWO WAT	629 630	-20.146 -21.707				
	ATOM	31	OWO WAT	631	-15.403				
г	MOTA	32	OWO WAT	632	-12.703				8
5	MOTA	33	OWO WAT	633	-12.479		39.250		8
	MOTA MOTA	34	OWO WAT	634	-13.921				8
	ATOM	35 36	OWO WAT	635 636	-7.230				8
	MOTA	37	OWO WAT	637	-2.989 -12.865				8
10	ATOM	38	OWO WAT	638	-2.754				8
	ATOM	39	OWO WAT	639	-17.416				8 8
	ATOM	40	OWO WAT	640	-31.068				8
	ATOM	41	OWO WAT	641	-17.725		21.261	1.00 25.43	8
15	ATOM ATOM	42 43	OWO WAT	642	-32.760				8
	ATOM	44	OWO WAT	643 644	-14.079 -16.644			1.00 20.23	8
	ATOM	45	OWO WAT	645	-1.790	22.930 38.223		1.00 34.00	8
	ATOM	46	OWO WAT	646	-10.026	24.026		1.00 30.63 1.00 31.10	8 8
20	MOTA	47	OWO WAT	647	-11.096	60.328	24.599	1.00 33.25	8
20	ATOM	48	OWO WAT	648	-19.457	27.850	-2.970	1.00 36.88	8
	MOTA MOTA	49	OWO WAT	649	-18.578	40.758	26.756	1.00 30.86	8
	ATOM	50 51	OWO WAT	650 651	-11.119	22.191	16.190	1.00 37.83	8
	ATOM		OWO WAT	651 652	-2.583 -0.243	24.179 25.713	28.032	1.00 73.18	8
25	ATOM		OWO WAT	653	-33.328	18.701	22.803 10.255	1.00 34.15 1.00 23.17	8
	ATOM	54	OWO WAT	654	-22.212	13.785	5.080	1.00 51.41	8 8
	ATOM		OWO WAT	655	-21.393	16.945	11.680	1.00 31.47	8
	ATOM ATOM		OWO WAT	656	-37.174	28.484	4.349	1.00 36.66	8
30	MOTA		OWO WAT	657	-23.291	46.916	13.981	1.00 45.02	8
	ATOM		OWO WAT	658 659	-31.521 -11.904	20.732 22.697	5.404	1.00 28.19	8
	ATOM	60	OWO WAT	660	-7.393	64.706	8.209 24.668	1.00 61.39 1.00 45.96	8
	ATOM	61	OWO WAT	661	-12.356	29.912	23.727	1.00 43.36	8 8
35	ATOM		TAW 0WO	662	-33.898	31.788	7.353	1.00 32.96	8
33	MOTA MOTA		TAW OWO	663	-28.502	48.102	25.478	1.00 58.40	8
	ATOM		TAW OWC	664 665	-23.414	63.056	18.427	1.00 35.16	8
	ATOM		OWO WAT	666	-4.792 -28.509	26.235 23.145	16.778	1.00 44.49	8
	ATOM		TAW OWC	667	-19.685	32.378	-1.620 -0.712	1.00 50.51 1.00 45.74	8 8
40	MOTA		TAW OWC	668	-10.899	26.379	23.620	1.00 43.74	8
	ATOM		TAW OWC	669	1.033	27.146	20.128	1.00 34.52	8
	ATOM ATOM		TAW OWC	670	-15.215	33.469	0.077	1.00 27.35	8
	ATOM		DWO WAT	671 672	-8.748 -22.332	20.877	16.508	1.00 51.59	8
45	ATOM		WO WAT	673	-23.373	18.552 30.095	3.707 17.610	1.00 30.25	8
	ATOM		WO WAT	674	-11.965	32.994	26.359	1.00 22.44 1.00 26.92	8 8
	ATOM		WO WAT	675	-35.793	29.720	7.198	1.00 27.19	8
	MOTA		WO WAT	676	-10.333	28.336	25.867	1.00 46.78	8
50	ATOM ATOM		WO WAT	677	-17.230	31.681	24.852	1.00 26.22	8
00	ATOM		WO WAT	678 679	-17.594	49.434	30.830	1.00 32.58	8
	MOTA	~~ ~	WO WAT	680	-8.561 -16.374	33.163 29.101	32.884 -4.195	1.00 37.04	8
	ATOM		WO WAT	681	-8.995	30.537	24.946	1.00 31.45 1.00 36.64	8 8
c r	ATOM		WO WAT	682	-19.019	53.815	28.676	1.00 48.06	8
55	ATOM		WO WAT	683	-20.039	39.516	15.742	1.00 23.23	8
	ATOM		WO WAT	684	-21.308	45.557	20.658	1.00 28.24	8
	ATOM ATOM		WO WAT WO WAT	685 686	-7.405	30.847	5.261	1.00 41.47	8
	ATOM		WO WAT	687	-23.729 -15.826	34.800 60.771	0.632	1.00 30.27	8
60	ATOM		WO WAT	688	0.119	50.495	23.946 24.812	1.00 41.94 0.50 25.93	8
	ATOM	89 O	WO WAT	689	-3.397	45.987	42.245	1.00 29.87	8 8
	MOTA		TAW OW	690	-10.215	47.715	32.270	1.00 43.33	8
	ATOM	91 0	WAT	691	-8.440	35.757	33.883	1.00 34.09	8
65	END								

TABLE 3

REMARK Homology model of Fc epsilon Receptor I by V. C. Epa; based on structure of FcgRIIa by K. Maxwell.

REMARK Produced by MODELLER: 24-Aug-98 01:02:51

	REM	ARK MO	DELLER	OBJECT	TIVE FUNC	TION:	643.1	1817			
5	ATO	M 1	N ·	VAL 1	36.4	42 43.25	2 22 10	4 1 0			
	ATO			VAL 1							SG
	ATO			VAL 1							SG .
	ATO		_		38.02						SG
10	ATO					51 41.57					SG (
10	ATO			/AL 1		14 42.50				15	
	ATON ATON			/AL 1			1 20.796			15	
	ATON			PRO 2						1.5	
	ATON			PRO 2 PRO 2	38.76					18	
15	ATOM		-	PRO 2	37.20					18	
	ATOM			RO 2	38.09 37.50					15	G 12
	ATOM	13		RO 2	38.75					1s	
	ATOM	14		RO 2	37.88					15	
20	MOTA		N G	LN 3	39.71					15	
20	ATOM			TN 3	39.78				0.19 0.19	15	
	ATOM			LN 3	40.95	1 41.913		1.00	0.19	1s:	
	ATOM ATOM			LN 3	41.17		14.092	1.00	0.19	150	
	ATOM			LN 3	42.43		13.369	1.00	0.19	150	
25	ATOM	21	OE1 G		42.83			1.00	0.19	150	
	ATOM	22		LN 3 LN 3	43.06			1.00	0.19	150	
	ATOM	23		LN 3	38.49° 37.82°			1.00	0.19	150	
	ATOM	24	N L		38.112			1.00	0.19	150	
20	ATOM	25	CA LY		36.855		13.932	1.00	0.23	150	
30	ATOM	26	CB L		36.146	44.354	13.776	1.00	0.23 0.23	186	
	ATOM	27	CG L		35.714	44.972	15.107	1.00	0.23	15G 15G	
	ATOM ATOM	28	CD L		35.315		14.996	1.00	0.23	15G	
	ATOM	29 30	CE LY		36.506		14.804	1.00	0.23	15G	
35	ATOM	31	C LY		36.033		14.631	1.00	0.23	1s _G	
	ATOM	32	O LY		37.089 37.990		12.560	1.00	0.23	1sg	
	ATOM	33	N PR		36.261		11.834	1.00	0.23	1sg	
	ATOM	34	CA PR		36.316		12.218 10.938	1.00	0.25	1SG	
40	ATOM	35	CD PR	0 5	34.937		12.804	1.00 1.00	0.25	1SG	
40	ATOM	36	CB PR		35.140		10.930	1.00	0.25 0.25	1SG 1SG	36 37
	ATOM	37	CG PR	-	34.094	40.656	11.780	1.00	0.25	15G	38
	MOTA MOTA	38 39	C PR		36.086	41.953	9.932	1.00	0.25	1SG	39
	ATOM		O PRO		35.464	42.958	10.275	1.00	0.25	1SG	40
45	ATOM		CA LY		36.592	41.786	8.699	1.00	0.35	1SG	41
	ATOM		CB LY		36.336	42.790	7.714	1.00	0.35	1SG	42
	ATOM		CG LYS		37.597 38.418	43.344 44.275	7.030		0.35	1SG	43
	ATOM		CD LYS		39.065	43.574	7.924 9.120	1.00	0.35	1SG	44
F.0	ATOM	45	CE LYS		39.884	44.516	10.004		0.35	1sg	45
50	ATOM		NZ LYS	6	40.469	43.767	11.137		0.35 0.35	15G	46
	ATOM		C LYS		35.491	42.168	6.659		0.35	1SG	47
	ATOM ATOM		O LYS		35.686	41.011	6.289		0.35	1SG 1SG	48 49
	ATOM		N VAL CA VAL		34.498	42.928	6.165		0.35	1sg	50
55	ATOM		CA VAL CB VAL	•	33.668	42.408	5.124		0.35	1s _G	51
	ATOM		CG1 VAL		32.207 32.014	42.721			0.35	1SG	52
	ATOM		G2 VAL		31.423	44.247 41.985			0.35	1SG	53
	ATOM	54 c			34.132	43.039			0.35	1s _G	54
C O	ATOM	55 C		7	34.313	44.254			0.35	1SG	55
60	ATOM	56 N	SER	8	34.363	42.211		1.00 (1.00 (0.35 0.17	15G	56
	ATOM		A SER	8	34.831	42.734).17	1SG 1SG	57
	ATOM		B SER	8	36.059	41.994			17	1SG	58 59
	ATOM ATOM		G SER	8	36.458		-0.210		17	15G	60
65	ATOM	60 C		8	33.733	42.575	0.586		.17	1SG	61
-	ATOM	62 N		8 9	33.030	41.566	0.575	L.00 0	.17	1SG	62
	ATOM	63 C		9	33.552 32.519				.11	1SG	63
	ATOM	64 C		9	31.563		-1.257 1		.11	1SG	64
70	ATOM	65 C		9	30.442				.11		65
70	MOTA		D2 LEU	9	29.725				.11		66
	ATOM	67 CI	D1 LEU	9					.11		67 69
						-			• • •	136	68

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ATOM 68 С LEU 9 33.175 43.554 -2.597 1.00 0.11 1SG ATOM 69 0 LEU 9 33.992 44.428 -2.883 1.00 0.11 1SG ATOM 70 N ASN 32.851 10 -3.450 42.565 1.00 0.17 1SG ATOM 71 CA ASN 10 33.401 42.565 -4.771 5 1.00 0.17 1SG MOTA 72 CB ASN 10 34.406 -5.011 41.428 1.00 0.17 1SG MOTA 73 CG ASN 10 35.623 41.693 -4.139 1.00 0.17 1SG ATOM 74 OD1 ASN 10 35.830 41.018 -3.132 1.00 0.17 1SG ATOM 75 ND2 ASN 10 -4.532 36.451 42.698 1.00 0.17 1SG MOTA 76 ASN С 10 32.257 42.340 -5.702 1.00 10 0.17 1SG ATOM 77 ASN 0 10 31.543 -5.585 41.346 1.00 0.17 1SG MOTA 78 N PRO 11 32.037 43.241 -6.615 1.00 0.35 1SG ATOM 79 CA PRO 11 -6.695 -7.923 32.836 44.431 1.00 0.35 1SG 80 MOTA 80 CD PRO 11 31.554 42.825 1.00 0.35 15G MOTA 81 81 CB PRO 11 32.565 45.023 -8.076 15 1.00 0.35 1SG 82 MOTA 82 CG PRO 11 32.180 43.803 -8.930 1.00 0.35 1\$G 83 MOTA 83 С PRO 11 32.450 45.345 -5.579 1.00 0.35 1s_G 84 MOTA 84 0 PRO 11 31.441 45.098 -4.920 1.00 0.35 1SG 8.5 MOTA 85 N PRO 12 33.234 46.363 -5.359 1.00 0.52 1SG MOTA 86 86 CA PRO 12 32.980 47.289 -4.289 1.00 0.52 20 1SG 87 MOTA 87 CD PRO 12 34.649 46.281 -5.684 1.00 0.52 1SG 88 ATOM 88 CB PRO 12 34.259 48.107 -4.134 1.00 0.52 1SG 89 ATOM 89 CG PRO 12 35.360 47.165 -4.647 1.00 0.52 1SG 90 MOTA 90 С PRO 12 31.775 48.132 -4.544 1.00 0.52 1SG 91 MOTA 91 0 PRO 12 31.347 48.837 -3.632 25 1.00 0.52 1SG 92 MOTA 92 N TRP 13 31.217 48.087 -5.767 1.00 0.35 1SG 93 MOTA 93 CA TRP 13 30.116 48.944 -6.099 1.00 0.35 MOTA 1SG 94 94 CB TRP 29.535 13 48.655 -7.492 1.00 0.35 1SG 95 ATOM 95 CG TRP 13 30.569 48.725 -8.590 1.00 0.35 1SG 96 ATOM 96 CD2 TRP 13 31.368 49.880 -8.883 1.00 30 0.35 1SG ATOM 97 97 CD1 TRP 13 30.982 47.743 -9.442 1.00 0.35 1SG 98 MOTA 98 NE1 TRP 31.981 48.216 -10.257 1.00 0.35 1SG 99 MOTA 99 CE2 TRP 13 32.232 49.530 -9.921 1.00 0.35 1SG 100 MOTA 100 CE3 TRP 13 31.389 51.127 -8.327 1.00 0.35 1SG 101 MOTA 101 CZ2 TRP 13 33.131 50.426 -10.422 1.00 0.35 35 1SG 102 MOTA 102 CZ3 TRP 13 32.292 52.032 -8.839 1.00 0.35 1SG 103 MOTA 103 CH2 TRP 13 33.145 51.687 -9.867 1.00 0.35 1SG 104 MOTA 104 TRP С 13 29.028 48.729 -5.094 1.00 0.35 1SG 105 MOTA 105 0 TRP 13 28.536 47.615 -4.920 1.00 0.35 1SG 106 MOTA 106 ASN 14 N 28.646 49.808 -4.379 40 1.00 0.15 1SG 107 MOTA 107 CA ASN 14 27.615 49.722 -3.385 1.00 0.15 1SG 108 MOTA 108 CB ASN 14 27.490 50.980 -2.504 1.00 0.15 1SG 109 ATOM 109 CG ASN 14 26.978 52.146 -3.340 1.00 0.15 1SG 110 MOTA 110 OD1 ASN 14 27.409 52.366 -4.471 1.00 0.15 1SG 111 ATOM 111 ND2 ASN 14 26.008 52.913 -2.773 1.00 45 0.15 1SG 112 MOTA 112 С ASN 14 26.300 49.521 -4.065 1.00 0.15 1SG 113 ATOM 113 0 ASN 14 25.463 48.747 -3.602 1.00 0.15 1SG 114 MOTA 114 N ARG 15 26.087 50.221 -5.196 1.00 0.13 1SG 115 MOTA 115 CA ARG 15 24.834 50.135 -5.884 1.00 0.13 1SG 116 MOTA CB 116 ARG 15 24.365 51.472 -6.487 1.00 50 0.13 1SG 117 MOTA 117 CG ARG -5.458 15 24.050 52.558 1.00 0.13 1SG 118 MOTA 118 CD ARG 15 23.590 53.872 -6.094 1.00 0.13 MOTA 1SG 119 119 NE ARG 15 23.349 54.844 -4.990 1.00 0.13 1SG 120 MOTA 120 CZARG 15 22.138 55.461 -4.864 1.00 0.13 1SG 121 ATOM 121 NH1 ARG 15 21.143 55.212 -5.764 1.00 0.13 55 MOTA 1SG 122 122 NH2 ARG 15 21.924 56.330 -3.833 1.00 0.13 1SG 123 MOTA 123 C ARG 15 25.033 49.218 -7.039 1.00 0.13 1SG 124 MOTA 124 0 ARG 15 25.976 49.374 -7.813 1.00 0.13 1SG 125 MOTA 125 ILE N 16 24.144 48.220 -7.185 1.00 0.12 1SG 126 MOTA 126 CA ILE 16 24.295 47.330 -8.294 1.00 60 0.12 1SG 127 ATOM 127 CB ILE 16 24.817 45.969 -7.928 1.00 0.12 1SG 128 MOTA CG2 ILE 128 16 26.224 46.139 -7.331 1.00 0.12 1SG 129 ATOM 129 CG1 ILE 16 23.828 45.237 -7.005 1.00 0.12 1SG 130 ATOM 130 CD1 ILE 16 24.141 43.749 1.00 -6.850 0.12 1SG 131 ATOM 131 С ILE 16 22.948 47.120 -8.892 1.00 0.12 65 1SG 132 ATOM 132 0 TTE 16 21.939 47.597 -8.374 1.00 0.12 1SG 133 ATOM 133 N PHE 17 22.919 46.404 -10.030 1.00 0.17 1SG 134 ATOM 134 CA PHE 17 21.684 46.108 -10.688 1.00 0.17 1SG 135 ATOM 135 CB PHE 17 21,755 46.075 -12.223 1.00 0.17 1SG 136 MOTA 136 CG PHE 47.447 -12.765 17 21.919 70 1.00 0.17 1SG 137 ATOM 137 CD1 PHE 17 20.844 48.303 -12.811 1.00 0.17 1SG 138 MOTA CD2 PHE 17 138 23.137 47.862 -13.248 1.00 0.17 1SG 139

	ATOM 139 CE1 PHE 1	.7 20.984 49.568 -13 324 1 00 0 17	
	ATOM 140 CE2 PHE 1	7 23.283 49.126 -13.764 1.00 0.17	1SG 140 1SG 141
		7 22.205 49.976 -13.800 1.00 0.17	1SG 141
5	ATOM 143 O PHE 1		1SG 143
	ATOM 144 N LYS 1 ATOM 145 CA LYS 1	8 20.018 44.402 -10.462 1.00 0.22	1SG 144 1SG 145
	ATOM 145 CA LYS 1 ATOM 146 CB LYS 1	8 18 040 43 043 10 162 1.00 0.22	1SG 146
10	ATOM 147 CG LYS 1		1SG 147
10	ATOM 148 CD LYS 1 ATOM 149 CE LYS 1	8 15.961 42.882 -11.672 1.00 0.22	1SG 148 1SG 149
	ATOM 149 CE LYS 1: ATOM 150 NZ LYS 1:	15.353 43.196 -13.039 1.00 0.22	1SG 150
	ATOM 151 C LYS 1	20.141 42.189 -11.210 1.00 0.22	1SG 151 1SG 152
15	ATOM 152 O LYS 16 ATOM 153 N GLY 19	20.335 42.596 -12.355 1.00 0.22	15G 152 1SG 153
	ATOM 154 CA GLY 19	20 986 40 005 11 757	1SG 154
	ATOM 155 C GLY 19 ATOM 156 O GLY 19	22.474 40.059 -11.692 1.00 0.21	1SG 155 1SG 156
	ATOM 156 O GLY 19 ATOM 157 N GLU 20	23.160 39.196 -12.236 1.00 0.21	1SG 157
20	ATOM 158 CA GLU 20		1SG 158
	ATOM 159 CB GLU 20 ATOM 160 CG GLU 20	24.940 42.579 -10.523 1.00 0.23	1SG 159 1SG 160
	ATOM 160 CG GLU 20 ATOM 161 CD GLU 20	24.680 43.613 -11.619 1.00 0.23	1SG 161
25	ATOM 162 OE1 GLU 20	26.556 42.653 -12.741 1.00 0.23	1SG 162
25	ATOM 163 OE2 GLU 20 ATOM 164 C GLU 20	24.774 43.175 -13.967 1.00 0.23	1SG 163 1SG 164
	ATOM 165 O GLU 20	24 122 30 806 0 004 1.00 0.23	1SG 165
	ATOM 166 N ASN 21	26.181 39.822 -9.930 1.00 0.16	1SG 166 1SG 167
30	ATOM 167 CA ASN 21 ATOM 168 CB ASN 21	26.694 38.898 -8.965 1.00 0.16	1SG 168
	ATOM 169 CG ASN 21	26 995 36 071 10 404	1SG 169
	ATOM 170 OD1 ASN 21 ATOM 171 ND2 ASN 21	25.671 36.909 -10.394 1.00 0.16	1SG 170 1SG 171
	ATOM 171 ND2 ASN 21 ATOM 172 C ASN 21	27.602 36.251 -11.392 1.00 0.16	1SG 172
35	ATOM 173 O ASN 21	27.415	1SG 173
	ATOM 174 N VAL 22 ATOM 175 CA VAL 22	27.217 39.327 -6.654 1.00 0.07	1SG 174 1SG 175
	ATOM 175 CA VAL 22 ATOM 176 CB VAL 22	27.876 40.026 -5.596 1.00 0.07 26.922 40.670 -4.632 1.00 0.07	1SG 176
40	ATOM 177 CG1 VAL 22	26.922 40.670 -4.632 1.00 0.07 27.727 41.288 -3.478 1.00 0.07	1SG 177 1SG 178
40	ATOM 178 CG2 VAL 22 ATOM 179 C VAL 22	26.056 41.681 -5.405 1.00 0.07	15G 178 15G 179
	ATOM 180 0 VAL 22	28.661 39.015 -4.836 1.00 0.07 28.186 37.907 -4.590 1.00 0.07	1SG 180
	ATOM 181 N THR 23 ATOM 182 CA THR 23	29.908 39.362 -4.469 1.00 0.06	1SG 181 1SG 182
45	ATOM 182 CA THR 23 ATOM 183 CB THR 23	30.692 38.440 -3.706 1.00 0.06	1SG 183
	ATOM 184 OG1 THR 23	31.980 38.047 -4.368 1.00 0.06 31.714 37.430 -5.619 1.00 0.06	1SG 184
	ATOM 185 CG2 THR 23 ATOM 186 C THR 23	32.727 37.067 -3.446 1.00 0.06	1SG 185 1SG 186
5 0	ATOM 186 C THR 23 ATOM 187 O THR 23	31.044 39.117 -2.425 1.00 0.06 31.577 40.225 -2.418 1.00 0.06	1SG 187
50	ATOM 188 N LEU 24	30.731 38.460 -1.295 1.00 0.06	1SG 188 1SG 189
	ATOM 189 CA LEU 24 ATOM 190 CB LEU 24	31.057 39.021 -0.020 1.00 0.06	1SG 190
	ATOM 191 CG LEU 24	20 702 20 020	1SG 191
55	ATOM 192 CD2 LEU 24 ATOM 193 CD1 LEU 24	29.182 41.346 0.123 1.00 0.06	1SG 192 1SG 193
	ATOM 193 CD1 LEU 24 ATOM 194 C LEU 24	27.548 39.924 1.495 1.00 0.06	1SG 194
	ATOM 195 O LEU 24	31 996 36 999 9 517	1SG 195
	ATOM 196 N THR 25 ATOM 197 CA THR 25	33.206 38.678 1.030 1.00 0.28	1SG 196 1SG 197
60	ATOM 197 CA THR 25 ATOM 198 CB THR 25	34.202 37.838 1.616 1.00 0.28	1SG 198
	ATOM 199 OG1 THR 25	35 310 37 412	1SG 199
	ATOM 200 CG2 THR 25	36.496 36.927 1.605 1.00 0.28	1SG 200 1SG 201
	ATOM 201 C THR 25 ATOM 202 O THR 25	34.460 38.367 2.979 1.00 0.28	1SG 202
65	ATOM 203 N CYS 26	24 543 27 460	1SG 203
	ATOM 204 CA CYS 26	34.770 37.922 5.286 1.00 0.52	1SG 204 1SG 205
	ATOM 205 CB CYS 26 ATOM 206 SG CYS 26	33.724 37.332 6.226 1.00 0.52	1SG 206
70	ATOM 207 C CYS 26		1SG 207
70	ATOM 208 0 CYS 26	36.327 36.201 5.748 1.00 0.52	1SG 208 1SG 209
	ATOM 209 N ASN 27	37 050 30 333 5 054	15G 209 1SG 210

	ATOM 210 CA ASN ATOM 211 CB ASN	27 38.377 37.91 27 39.472 38.67	1120 1100 0.33	1SG 211 1SG 212
5	ATOM 212 CG ASN ATOM 213 OD1 ASN ATOM 214 ND2 ASN	27 39.389 40.14 27 38.320 40.74	0 5.927 1.00 0.35 7 5.897 1.00 0.35	1SG 212 1SG 213 1SG 214
Ŭ	ATOM 215 C ASN	27 40.549 40.72 27 38.595 38.21	6 6.326 1.00 0.35 1 7.743 1.00 0.35	1SG 215 1SG 216
	ATOM 217 N GLY	27 37.972 39.10 ^o 28 39.483 37.42 ^o	7 8.310 1.00 0.35 7 8.381 1.00 0.15	1SG 217 1SG 218
10	ATOM 219 C GLY	28 39.779 37.630 28 40.251 36.330	6 9.765 1.00 0.15 0 10.306 1.00 0.15	1SG 219 1SG 220
	ATOM 221 N ASN	28 40.302 35.333 29 40.604 36.29	9.587 1.00 0.15 11.606 1.00 0.16	1SG 221 1SG 222
15	ATOM 223 CB ASN	29 41.053 35.065 29 41.554 35.176	5 12.173 1.00 0.16 5 13.624 1.00 0.16	1SG 223 1SG 224
15	ATOM 224 CG ASN ATOM 225 OD1 ASN	29 42.895 35.895 29 43.494 36.131	13.621 1.00 0.16	1SG 225 1SG 226
	ATOM 226 ND2 ASN ATOM 227 C ASN	29 43.391 36.241 29 39.883 34.143	14.838 1.00 0.16	1SG 227 1SG 228
20	ATOM 229 N ASN	29 38.741 34.566 30 40.148 32.843	12.336 1.00 0.16 11.949 1.00 0.16	15G 229 1SG 230
	ATOM 231 CB ASN	30 39.080 31.893 30 38.855 31.359	11.889 1.00 0.16	1SG 231 1SG 232
25	ATOM 233 OD1 ASN	30 37.718 30.355 30 36.716 30.535	10.511 1.00 0.16 11.200 1.00 0.16	1SG 232 1SG 233 1SG 234
23	ATOM 235 C ASN :	30 37.899 29.239 30 39.436 30.721	9.758 1.00 0.16 12.744 1.00 0.16	1SG 234 1SG 235 1SG 236
	ATOM 237 N PHE	30 40.609 30.390 31 38.409 30.073	12.909 1.00 0.16 13.332 1.00 0.12	1SG 237 1SG 238
30	ATOM 239 CB PHE	31 38.628 28.899 31 37.510 28.639	14.123 1.00 0.12 15.146 1.00 0.12	15G 239 1SG 240
	ATOM 241 CD1 PHE	31 37.857 27.404 31 38.774 27.447	15.902 1.00 0.12 16.927 1.00 0.12	1SG 241 1SG 242
35	ATOM 243 CE1 PHE 3	31 37.260 26.205 31 39.092 26.310	15.592 1.00 0.12 17.631 1.00 0.12	1SG 243 1SG 244
	ATOM 245 CZ PHE 3	31 37.575 25.064 31 38.495 25.115	16.292 1.00 0.12 17.312 1.00 0.12	1SG 245 1SG 246
	ATOM 247 0 PHE 3	38.639 27.765 38.118 27.888 2 39.248 26.626	13.155 1.00 0.12 12.049 1.00 0.12	1SG 247 1SG 248
40	ATOM 249 CA PHE 3	2 39.265 25.565	13.528 1.00 0.11 12.570 1.00 0.11	1SG 249 1SG 250
	ATOM 251 CG PHE 3 ATOM 252 CD1 PHE 3		12.773 1.00 0.11 12.563 1.00 0.11	1SG 251 1SG 252
45	ATOM 253 CD2 PHE 3. ATOM 254 CE1 PHE 3.	2 42.284 25.417	13.602 1.00 0.11 11.337 1.00 0.11	1SG 253 1SG 254
	ATOM 255 CE2 PHE 33 ATOM 256 CZ PHE 33	2 43.424 26.164	13.428 1.00 0.11 11.157 1.00 0.11	1SG 255 1SG 256
	ATOM 257 C PHE 32 ATOM 258 O PHE 32	2 37.980 24.827	12.201 1.00 0.11 12.710 1.00 0.11	1SG 257 1SG 258
50	ATOM 259 N GLU 33 ATOM 260 CA GLU 33	36.949 25.287	13.460 1.00 0.11 11.977 1.00 0.10	1SG 259 1SG 260
	ATOM 261 CB GLU 33 ATOM 262 CG GLU 33	34.682 25.327	12.038 1.00 0.10 12.994 1.00 0.10	1SG 261 1SG 262
55	ATOM 263 CD GLU 33 ATOM 264 OE1 GLU 33	33.383 27.314	12.610 1.00 0.10 13.638 1.00 0.10	1SG 263 1SG 264
	ATOM 265 OE2 GLU 33 ATOM 266 C GLU 33	33.567 28.481	13.999 1.00 0.10 14.077 1.00 0.10	1SG 265 1SG 266
	ATOM 267 O GLU 33 ATOM 268 N VAL 34	35.453 25.532	10.672 1.00 0.10 9.849 1.00 0.10	1SG 267 1SG 268
60	ATOM 269 CA VAL 34 ATOM 270 CB VAL 34	33.509 23.763	10.391 1.00 0.09 9.103 1.00 0.09	1SG 269 1SG 270
	ATOM 271 CG1 VAL 34 ATOM 272 CG2 VAL 34	31.945 22.676	8.943 1.00 0.09 7.538 1.00 0.09	1SG 271 1SG 272
65	ATOM 273 C VAL 34 ATOM 274 O VAL 34	32.742 25.032 32.854 25.693	9.215 1.00 0.09 8.926 1.00 0.09	1SG 273 1SG 274
	ATOM 275 N SER 35 ATOM 276 CA SER 35	31.953 25.431 31.202 26.645	7.895 1.00 0.09 9.942 1.00 0.11	1SG 275 1SG 276
	ATOM 277 CB SER 35 ATOM 278 OG SER 35	29.838 26.613 1	9.800 1.00 0.11 10.522 1.00 0.11	1SG 277 1SG 278
70	ATOM 279 C SER 35 ATOM 280 O SER 35	32.033 27.743 1	11.915 1.00 0.11 10.378 1.00 0.11	1SG 279 1SG 280
		01.000 28.133 1	1.524 1.00 0.11	1SG 281

	ATOM 281 N SER 3	6 32.974 28.249	9.563 1.00 0.27	
	ATOM 282 CA SER 3 ATOM 283 CB SER 3	6 33.906 29.251	9.984 1.00 0.27	1SG 282 1SG 283
5	ATOM 284 OG SER 3	6 35.648 28.343	8.905 1.00 0.27 8.571 1.00 0.27	1SG 284 1SG 285
•	ATOM 286 O SER 3		10.256 1.00 0.27	1SG 286
	ATOM 287 N THR 3 ATOM 288 CA THR 3	7 32.290 30.954	9.360 1.00 0.48	1SG 287 1SG 288
10	ATOM 289 CB THR 3	32.132 33.216	9.550 1.00 0.48 8.462 1.00 0.48	1SG 289
10	ATOM 290 OG1 THR 3' ATOM 291 CG2 THR 3'		8.737 1.00 0.48	1SG 290 1SG 291
	ATOM 292 C THR 3	30.265 32.253	7.124 1.00 0.48 9.596 1.00 0.48	1SG 292 1SG 293
1 5	ATOM 294 N LYS 38		9.105 1.00 0.48	1SG 294
15	ATOM 295 CA LYS 38 ATOM 296 CB LYS 38	28.291 33.482	10.294 1.00 0.41	1SG 295 1SG 296
	ATOM 297 CG LYS 38	27.770 33.754 28.245 32.739	11.715 1.00 0.41 12.757 1.00 0.41	1SG 297 1SG 298
0.0	ATOM 298 CD LYS 38 ATOM 299 CE LYS 38	29.734 32.877 30.193 32.030	13.087 1.00 0.41	1SG 298
20	ATOM 300 NZ LYS 38	31.621 32.301	14.276 1.00 0.41 14.565 1.00 0.41	1SG 300 1SG 301
	ATOM 302 0 LYS 38	28.013 34.720 28.709 35.726	9.506 1.00 0.41	1SG 302
	ATOM 303 N TRP 39 ATOM 304 CA TRP 39	26.998 34.677	8.624 1.00 0.18	1SG 303 1SG 304
25	ATOM 305 CB TRP 39	26.680 35.852 26.599 35.645	7.870 1.00 0.18 6.344 1.00 0.18	1SG 305
	ATOM 306 CG TRP 39 ATOM 307 CD2 TRP 39	27.940 35.495	5.663 1.00 0.18	1SG 306 1SG 307
	ATOM 308 CD1 TRP 39	28.585 34.378	5.377 1.00 0.18 5.220 1.00 0.18	1SG 308 1SG 309
30	ATOM 309 NE1 TRP 39 ATOM 310 CE2 TRP 39	29.800 34.725 29.947 36.094	4.672 1.00 0.18	1SG 310
	ATOM 311 CE3 TRP 39	28.656 37.943	4.764 1.00 0.18 5.611 1.00 0.18	1SG 311 1SG 312
	ATOM 313 CZ3 TRP 39	30.964 36.918 29.681 38.772	4.374 1.00 0.18	1SG 313
35	ATOM 314 CH2 TRP 39 ATOM 315 C TRP 39	30.813 38.269	4.607 1.00 0.18	1SG 314 1SG 315
	ATOM 316 O TRP 39	24.473 35.536	8.319 1.00 0.18 8.668 1.00 0.18	1SG 316 1SG 317
	ATOM 317 N PHE 40 ATOM 318 CA PHE 40	25.166 37.662 23.898 38.177	8.355 1.00 0.08	1SG 318
40	ATOM 319 CB PHE 40	23.942 38.924 1	8.759 1.00 0.08 10.102 1.00 0.08	1SG 319 1SG 320
	ATOM 321 CD1 PHE 40		11.142 1.00 0.08 11.393 1.00 0.08	1SG 321
	ATOM 322 CD2 PHE 40 ATOM 323 CE1 PHE 40	23.262 37.311 1	1.865 1.00 0.08	1SG 322 1SG 323
45	ATOM 324 CE2 PHE 40	23.555 36.372 1	2.352 1.00 0.08 2.826 1.00 0.08	1SG 324 1SG 325
	ATOM 326 C PHE 40		3.071 1.00 0.08	1SG 326
	ATOM 327 O PHE 40 ATOM 328 N HIS 41	24.243 39.920	7.189 1.00 0.08	1SG 327 1SG 328
50	ATOM 329 CA HIS 41		7.382 1.00 0.10 6.468 1.00 0.10	1SG 329
30	ATOM 330 ND1 HIS 41 ATOM 331 CG HIS 41	19.882 40.132	3.044 1.00 0.10	1SG 330 1SG 331
	ATOM 332 CB HIS 41	20.942 39.397	4.242 1.00 0.10 5.232 1.00 0.10	15G 332 15G 333
	ATOM 333 NE2 HIS 41 ATOM 334 CD2 HIS 41	20.036 42.349	3.153 1.00 0.10	1SG 334
55	ATOM 335 CE1 HIS 41	19.631 41.317 2	4.294 1.00 0.10 2.434 1.00 0.10	1SG 335 1SG 336
	ATOM 337 O HIS 41		7.226 1.00 0.10	1SG 337
	ATOM 338 N ASN 42 ATOM 339 CA ASN 42	20.632 42.049	7.386 1.00 0.11	1SG 338 1SG 339
60	ATOM 340 CB ASN 42	10 000 10	3.132 1.00 0.11 7.489 1.00 0.11	1SG 340
	ATOM 341 CG ASN 42 ATOM 342 OD1 ASN 42	18.291 43.691 6	.283 1.00 0.11	1SG 341 1SG 342
	ATOM 343 ND2 ASN 42		.062 1.00 0.11 .492 1.00 0.11	1SG 343 1SG 344
65	ATOM 344 C ASN 42 ATOM 345 O ASN 42	19.566 42.155 9	.490 1.00 0.11	1SG 345
	ATOM 346 N GLY 43	20.683 41.567 9	.144 1.00 0.11 .955 1.00 0.08	1SG 346 1SG 347
	ATOM 348 C GLY 43	20.714 41.014 11	.277 1.00 0.08	1SG 348
70	ATOM 349 O GLY 43	20.036 39.001 12.	.264 1.00 0.08 .318 1.00 0.08	1SG 349 1SG 350
· =	ATOM 350 N SER 44 ATOM 351 CA SER 44		.079 1.00 0.15	1SG 351
		10,	.068 1.00 0.15	1SG 352

ATOM 353 Go Ser 44		ATO	M 352	2 CB	SER	44	18.2	18 37.4	98 9.0	24 1 4	00 0 15	
ATOM 355							18.73	37 37.6	41 7.7			1SG 353 1SG 354
ATOM 355 CA LEU 45 20.638 35.747 10.491 1.00 0.35 186 357	-							. .				1SG 355
ATOM 358 CB LEU 46 21,929 33,8483 10,241 1,00 0,35 18G 358 ATOM 360 CD2 LEU 45 22,938 33,852 11,258 1,00 0,35 18G 358 ATOM 361 CD1 LEU 45 22,938 31,852 11,258 1,00 0,35 18G 369 ATOM 361 CD1 LEU 45 22,938 31,862 11,258 1,00 0,35 18G 369 ATOM 362 C LEU 45 22,398 31,682 11,258 1,00 0,35 18G 361 ATOM 363 O LEU 45 22,398 31,682 11,258 1,00 0,35 18G 361 ATOM 365 CR SER 46 22,435 31,186 81,133 1,00 0,35 18G 363 ATOM 365 CR SER 46 22,455 31,186 81,133 1,00 0,38 18G 363 ATOM 367 CR SER 46 22,355 31,186 81,38 1,00 0,48 18G 365 ATOM 369 CR SER 46 22,355 31,198 61,398 1,00 0,48 18G 365 ATOM 373 CR GLU 47 22,721 30,711 6,936 1,00 0,48 18G 369 ATOM 373 CR GLU 47 22,721 30,711 6,936 1,00 0,48 18G 369 ATOM 373 CR GLU 47 22,721 30,711 6,936 1,00 0,44 18G 372 ATOM 373 CR GLU 47 22,721 30,711 6,936 1,00 0,44 18G 372 ATOM 375 CR GLU 47 19,700 27,272 29,311 7,017 1,00 0,48 18G 374 ATOM 375 CR GLU 47 19,700 27,272 29,311 7,00 0,44 18G 372 ATOM 375 CR GLU 47 19,700 27,272 29,311 7,00 0,44 18G 372 ATOM 375 CR GLU 47 19,539 26,690 6,845 1,00 0,44 18G 374 ATOM 377 C GLU 47 24,413 28,215 5,800 1,00 0,44 18G 374 ATOM 378 CR GLU 47 19,539 26,690 6,845 1,00 0,44 18G 374 ATOM 378 CR GLU 47 19,539 26,690 6,845 1,00 0,44 18G 374 ATOM 378 CR GLU 48 23,741 29,635 33,877 0,00 0,44 18G 374 ATOM 378 CR GLU 48 23,748 28,215 5,800 1,00 0,44 18G 374 ATOM 388 CR GLU 48 23,748 29,158 47,30 1,00 0,45 18G 383 ATOM 389 CR GRU 48 23,748 32,140 2,925 1,00 0,45 18G 383 ATOM 380 CR GRU 48 23,748 29,138 2,100 0,45 18G 383 ATOM 380 CR GRU 48 23,748 29,138 2,100 0,45 18G 383 ATOM 380 CR GRU 48 23,748 29,138 2,100 0,45 18G 383 ATOM 380 CR GRU 48 23,748 29,138 2,100 0,45 18G 383 ATOM 380 CR GRU 48 23,748 29,138 2,100 0,45 18G 383 ATOM 380 CR GRU 48 23,748 29,138 2,100 0,45 18G 383 ATOM 380 CR GRU 48 23,748 29,138 2,100 0,45 18G 383 ATOM 380 CR GRU 48 23,748 29,138 29,100 0,45 18G 383 ATOM 380 CR GRU 48 23,748 29,138 29,100 0,45 18G 383 ATOM 380 CR GRU 48 23,748 29,138 29,100 0,45 18G 383 ATOM 38	5						20.63	38 35.7				
10 ARCH 359 C C LEU 45 22.991 32.283 11.298 1.00 0.35 18S 360 ARCH 361 CD1 LEU 45 22.938 31.865 10.100 1.00 0.35 18S 360 ARCH 362 C LEU 45 22.938 31.865 10.100 1.00 0.35 18S 360 ARCH 362 C LEU 45 22.938 31.865 10.100 1.00 0.35 18S 360 ARCH 362 C LEU 45 21.398 31.695 10.100 1.00 0.35 18S 360 ARCH 362 C LEU 45 21.398 31.695 10.100 1.00 0.35 18S 360 ARCH 362 C LEU 45 21.398 31.695 10.100 1.00 0.35 18S 360 ARCH 362 AR							21.72	20 34.8			0.35	1SG 358
10				CG	LEU	45						
ATOM 362 C LEU 45 20.1398 34.007 12.802 1.00 0.35 136 363 136 370 LEU 45 20.249 33.730 8.988 1.00 0.45 136 365 136 136	10								65 10.1	00 1.0	0.35	
ATOM 363 0 LEU 45 20.249 33.736 8.740 1.00 0.35 180 364 180 36		ATOM	3 62	С								
ATOM 365 CA SER 46 22.263 33.118 6.938 1.00 0.48 186 366 CA CA CA CA CA CA CA							20.24	9 33.73	86 8.7			
ATOM 366 CB SER 46	• •											1SG 365
20 ATOM 366 C SER 46 22.355 34.958 3.34 1.00 0.48 ISG 368 ATOM 369 C SER 46 24.137 31.770 7.487 1.00 0.48 ISG 369 ATOM 370 N GUU 47 22.724 29.371 7.026 1.00 0.44 ISG 370 ATOM 371 CA GUU 47 22.724 29.371 7.027 1.00 0.44 ISG 370 ATOM 373 C G GUU 47 20.768 28.350 5.745 1.00 0.44 ISG 371 ATOM 373 C G GUU 47 20.768 28.350 5.745 1.00 0.44 ISG 371 ATOM 373 C G GUU 47 19.559 26.690 6.945 1.00 0.44 ISG 371 ATOM 376 C GUU 47 19.559 26.690 6.945 1.00 0.44 ISG 376 ATOM 377 C GUU 47 19.559 26.690 6.945 1.00 0.44 ISG 376 ATOM 377 C GUU 47 19.559 26.690 6.945 1.00 0.44 ISG 376 ATOM 378 C GUU 47 23.552 29.092 5.809 1.00 0.44 ISG 376 ATOM 378 C GUU 47 23.552 29.092 5.800 1.00 0.44 ISG 376 ATOM 378 C GUU 48 23.781 29.858 1.00 0.44 ISG 378 ATOM 378 C GUU 48 23.781 29.858 1.00 0.44 ISG 378 ATOM 378 C GUU 48 23.781 29.858 1.00 0.44 ISG 378 ATOM 378 C GUU 48 23.789 23.245 29.858 1.00 0.44 ISG 378 ATOM 378 C GUU 48 23.789 23.245 29.858 1.00 0.45 ISG 380 ATOM 380 CA GUU 48 23.187 33.215 2.041 1.00 0.45 ISG 380 ATOM 380 CA GUU 48 23.187 33.215 2.041 1.00 0.45 ISG 382 ATOM 385 C G GUU 48 23.187 33.215 2.041 1.00 0.45 ISG 382 ATOM 385 C G GUU 48 23.459 34.417 2.302 1.00 0.45 ISG 382 ATOM 388 C G GUU 48 23.459 34.417 2.302 1.00 0.45 ISG 384 ATOM 387 C G GUU 48 23.459 34.417 2.302 1.00 0.45 ISG 386 ATOM 388 N AT HR 49 26.867 30.365 3.758 1.00 0.55 ISG 381 ATOM 389 C A THR 49 27.427 30.251 3.324 1.00 0.55 ISG 389 ATOM 389 C A THR 49 27.427 30.251 3.324 1.00 0.55 ISG 389 ATOM 399 C B THR 49 27.427 30.551 3.324 1.00 0.55 ISG 389 ATOM 399 C B THR 49 27.427 30.551 3.324 1.00 0.55 ISG 399 ATOM 399 C B THR 49 27.427 30.551 3.324 1.00 0.55 ISG 399 ATOM 399 C B ATOM 399 C B ASN 50 31.925 28.990 4.291 1.00 0.44 ISG 399 ATOM 399 C B ASN 50 31.935 27.665 4.747 1.00 0.44 ISG 399 ATOM 399 C B ASN 50 31.325 3.324 3.327 1.00 0.55 ISG 399 ATOM 399 C B ASN 50 31.325 3.324 3.327 1.00 0.55 ISG 399 ATOM 400 NN 2 ASN 50 31.325 4.329 1.00 0.44 ISG 399 ATOM 400 NN 2 ASN 50 31.325 4.329 1.00 0.25 ISG 408 ATOM 400 NN 2 ASN 50 31.325 3.3290 4.429 1.00 0.25 ISG 408 A	15						22.95	7 33.73	0 5.70			
20 ATOM 369 O SER 46								_			0 0.48	1SG 368
20 ALOM 371 CA GLU 47 22.221 30.711 6.936 1.00 0.44 18G 371 ATOM 372 CB GLU 47 21.604 28.321 7.026 1.00 0.44 18G 373 ATOM 373 CG GLU 47 21.604 28.321 7.026 1.00 0.44 18G 373 ATOM 373 CG GLU 47 19.708 27.272 5.839 1.00 0.44 18G 373 ATOM 375 CB GLU 47 19.709 27.272 5.839 1.00 0.44 18G 375 ATOM 375 CB GLU 47 19.509 26.609 6.945 1.00 0.44 18G 375 ATOM 376 CB GLU 47 19.509 26.609 6.945 1.00 0.44 18G 375 ATOM 377 C GLU 47 21.612 29.295 5.800 1.00 0.44 18G 375 ATOM 378 N GLU 47 22.286 29.858 4.730 1.00 0.44 18G 376 ATOM 378 N GLU 48 23.741 29.635 3.387 1.00 0.44 18G 376 ATOM 378 N GLU 48 23.741 29.635 3.387 1.00 0.44 18G 378 ATOM 378 N GLU 48 23.741 29.635 3.387 1.00 0.45 18G 388 ATOM 383 CB GLU 48 23.741 29.635 3.387 1.00 0.45 18G 388 ATOM 383 CD GLU 48 23.749 32.140 29.635 3.00 0.45 18G 388 ATOM 383 CD GLU 48 23.789 32.140 29.852 1.00 0.45 18G 382 ATOM 386 CB GLU 48 23.789 32.140 29.852 1.00 0.45 18G 384 ATOM 386 CB GLU 48 23.499 34.417 30.00 0.45 18G 386 ATOM 386 CB GLU 48 23.499 34.417 30.00 0.45 18G 386 ATOM 386 CB GLU 48 23.499 34.417 30.00 0.45 18G 386 ATOM 386 CB GLU 48 25.226 29.496 3.195 1.00 0.45 18G 386 ATOM 388 N THR 49 26.087 30.365 3.758 1.00 0.45 18G 386 ATOM 389 CA THR 49 27.684 31.365 1.00 0.45 18G 386 ATOM 390 CB THR 49 22.684 30.361 3.156 1.00 0.45 18G 386 ATOM 390 CB THR 49 27.684 31.365 1.00 0.55 18G 399 ATOM 399 CG THR 49 27.629 32.679 2.988 1.00 0.55 18G 399 ATOM 399 CG THR 49 27.629 32.679 2.986 1.00 0.55 18G 399 ATOM 399 CD ATOM 400 ND2 ASN 50 31.935 26.930 4.291 1.00 0.44 18G 399 ATOM 400 ND2 ASN 50 31.935 26.930 4.291 1.00 0.44 18G 399 ATOM 400 ND2 ASN 50 31.935 26.930 4.291 1.00 0.44 18G 399 ATOM 400 ND2 ASN 50 31.935 26.930 4.291 1.00 0.44 18G 399 ATOM 400 ND2 ASN 50 31.935 26.930 4.291 1.00 0.44 18G 399 ATOM 400 ND2 ASN 50 31.935 26.930 4.291 1.00 0.44 18G 399 ATOM 400 ND2 ASN 50 31.935 26.930 4.291 1.00 0.44 18G 399 ATOM 400 ND2 ASN 50 31.935 26.930 4.291 1.00 0.44 18G 399 ATOM 400 ND2 ASN 50 31.938 31.255 4.3291 1.00 0.55 18G 399 ATOM 400 ND2 ASN 50 31.938 31.255 4.3291 1.00 0.25 18G 4					SER	46	24.13	7 31.77				
ATOM 372 CB GLU 47 21.604 22.321 7.026 1.00 0.44 1SG 373 ATOM 374 CD GLU 47 19.539 26.690 6.945 1.00 0.44 1SG 375 ATOM 375 OEI GLU 47 19.539 26.690 6.945 1.00 0.44 1SG 375 ATOM 376 OEI GLU 47 19.539 26.690 6.945 1.00 0.44 1SG 375 ATOM 378 O GLU 47 23.552 29.092 5.800 1.00 0.44 1SG 375 ATOM 378 O GLU 47 23.552 29.092 5.800 1.00 0.44 1SG 375 ATOM 378 O GLU 48 23.244 13 28.215 5.800 1.00 0.44 1SG 375 ATOM 378 O GLU 48 23.244 13 28.215 5.800 1.00 0.44 1SG 379 ATOM 378 O GLU 48 23.244 13 28.215 5.800 1.00 0.45 1SG 389 ATOM 381 CB GLU 48 23.244 13 28.215 5.800 1.00 0.45 1SG 389 ATOM 382 CG GLU 48 23.284 30.775 2.465 1.00 0.45 1SG 381 ATOM 383 CD GLU 48 23.284 30.775 2.465 1.00 0.45 1SG 381 ATOM 385 OEZ GLU 48 23.284 30.775 2.465 1.00 0.45 1SG 382 ATOM 385 OEZ GLU 48 23.284 30.775 2.465 1.00 0.45 1SG 382 ATOM 385 OEZ GLU 48 23.284 30.775 2.465 1.00 0.45 1SG 382 ATOM 385 OEZ GLU 48 23.284 30.775 2.465 1.00 0.45 1SG 382 ATOM 385 OEZ GLU 48 23.284 30.775 2.465 1.00 0.45 1SG 382 ATOM 385 OEZ GLU 48 23.187 33.215 2.041 1.00 0.45 1SG 382 ATOM 385 OEZ GLU 48 23.459 34.417 2.302 1.00 0.45 1SG 382 ATOM 380 C G GLU 48 23.549 24.60 3.155 1.00 0.45 1SG 386 ATOM 380 C G GLU 48 23.459 34.417 2.302 1.00 0.45 1SG 386 ATOM 380 C G GLU 48 23.65 31 31.55 1.00 0.45 1SG 386 ATOM 380 C G GLU 48 23.65 31 31.55 1.00 0.45 1SG 388 ATOM 380 C G GLU 48 25.647 29.456 3.155 1.00 0.45 1SG 388 ATOM 380 C G GLU 48 25.647 30.365 3.758 1.00 0.55 1SG 389 ATOM 380 C G GLU 48 25.647 30.365 3.758 1.00 0.55 1SG 389 ATOM 380 C G GLU 48 25.647 30.365 3.758 1.00 0.55 1SG 389 ATOM 380 C G GLU 48 25.647 30.365 3.758 1.00 0.55 1SG 389 ATOM 380 C G GLU 48 25.647 30.365 3.758 1.00 0.55 1SG 389 ATOM 380 C G GLU 48 25.647 30.365 3.758 1.00 0.55 1SG 389 ATOM 380 C G GLU 48 25.647 30.365 3.758 1.00 0.55 1SG 389 ATOM 380 C G GLU 48 25.647 30.365 3.758 1.00 0.55 1SG 389 ATOM 380 C G ASN 50 31.335 27.665 1.747 1.00 0.55 1SG 389 ATOM 380 C G ASN 50 31.335 27.665 1.747 1.00 0.55 1SG 389 ATOM 380 C G ASN 50 31.335 27.665 1.747 1.00 0.55 1SG 389 ATOM 380 C G ASN 50 31.335 32.	20								1 6.93	6 1.0	0 0.44	
ATOM 373 CG GLU 47 20.768 28.350 5.745 1.00 0.44 18G 374 ATOM 375 OEI GLU 47 19.539 26.690 6.945 1.00 0.44 18G 376 ATOM 376 OEZ GLU 47 19.539 26.690 6.945 1.00 0.44 18G 376 ATOM 377 C GLU 47 23.552 29.992 5.800 1.00 0.44 18G 376 ATOM 378 O GLU 48 23.258 29.992 5.800 1.00 0.44 18G 376 ATOM 378 O GLU 48 23.258 29.992 5.800 1.00 0.44 18G 378 ATOM 378 O GLU 48 23.268 29.968 4.730 1.00 0.45 18G 378 ATOM 381 CB GLU 48 23.2741 29.635 4.700 1.00 0.45 18G 380 ATOM 381 CB GLU 48 23.2741 29.635 4.700 1.00 0.45 18G 380 ATOM 382 CG GLU 48 23.2741 29.635 3.387 1.00 0.45 18G 382 ATOM 383 CD GLU 48 23.187 33.215 2.0411 1.00 0.45 18G 382 ATOM 383 CD GLU 48 23.478 32.140 2.929 1.00 0.45 18G 382 ATOM 385 OEZ GLU 48 23.459 34.417 2.302 1.00 0.45 18G 382 ATOM 385 OEZ GLU 48 23.459 34.417 2.302 1.00 0.45 18G 386 ATOM 385 OEZ GLU 48 23.459 34.417 2.302 1.00 0.45 18G 386 ATOM 388 N THR 49 26.087 30.365 3.758 1.00 0.45 18G 386 ATOM 389 CA THR 49 27.629 30.365 3.758 1.00 0.45 18G 386 ATOM 389 CA THR 49 27.629 30.365 3.758 1.00 0.55 18G 390 ATOM 399 CA THR 49 27.629 32.679 2.968 1.00 0.55 18G 390 ATOM 399 CA THR 49 27.629 32.679 2.968 1.00 0.55 18G 392 ATOM 391 CO THR 49 27.629 32.679 2.968 1.00 0.55 18G 392 ATOM 393 C THR 49 28.213 30.658 5.473 1.00 0.55 18G 393 ATOM 393 C THR 49 28.23 30.690 3.881 1.00 0.55 18G 393 ATOM 393 C THR 49 28.23 30.690 3.881 1.00 0.55 18G 393 ATOM 393 C THR 49 28.213 30.658 5.473 1.00 0.55 18G 393 ATOM 393 C THR 49 28.213 30.658 5.473 1.00 0.55 18G 393 ATOM 399 CA AND 398 CA AND 50 30.937 30.109 4.665 1.00 0.44 18G 389 ATOM 390 CA AND 50 30.937 30.109 4.665 1.00 0.44 18G 389 ATOM 390 CA AND 50 30.937 30.109 4.665 1.00 0.44 18G 389 ATOM 390 CA AND 50 30.937 30.109 4.665 1.00 0.44 18G 389 ATOM 390 CA AND 50 30.937 30.109 4.665 1.00 0.44 18G 389 ATOM 400 NDZ AND 50 31.032 2.7665 4.747 1.00 0.44 18G 389 ATOM 400 NDZ AND 50 31.032 2.7665 4.747 1.00 0.44 18G 389 ATOM 400 NDZ AND 50 31.032 2.7665 4.747 1.00 0.44 18G 389 ATOM 400 NDZ AND 50 31.032 2.7765 31.247 1.00 0.25 18G 401 ATOM 410 C A SER 51 33.3843 32.247 4.3		ATOM	372	СВ	GLU							
25 ATOM 376 OEL GLU 47 19.030 27.016 4.803 1.00 0.44 15G 376 ATOM 377 C GLU 47 19.030 27.016 4.803 1.00 0.44 15G 376 ATOM 378 O GLU 47 24.413 28.215 5.800 1.00 0.44 15G 378 ATOM 379 N GLU 48 23.268 29.658 4.730 1.00 0.44 15G 378 ATOM 379 N GLU 48 23.741 29.635 3.387 1.00 0.45 15G 380 ATOM 381 CB GLU 48 23.741 29.635 3.387 1.00 0.45 15G 380 ATOM 381 CB GLU 48 23.741 29.635 3.387 1.00 0.45 15G 380 ATOM 382 CG GLU 48 23.788 32.140 29.91 1.00 0.45 15G 383 ATOM 382 CG GLU 48 23.789 32.140 29.91 1.00 0.45 15G 383 ATOM 384 OEL GLU 48 22.440 32.852 1.00 0.45 15G 383 ATOM 385 OEZ GLU 48 22.459 34.417 2.302 1.00 0.45 15G 383 ATOM 386 C GLU 48 25.266 29.496 3.155 1.00 0.45 15G 383 ATOM 386 C GLU 48 25.266 29.496 3.155 1.00 0.45 15G 386 ATOM 380 N THR 49 25.667 29.496 3.155 1.00 0.45 15G 386 ATOM 380 N THR 49 25.667 29.496 3.155 1.00 0.45 15G 386 ATOM 380 N THR 49 27.427 30.251 0.00 0.45 15G 386 ATOM 380 N THR 49 27.627 30.251 3.247 1.00 0.55 15G 389 ATOM 380 N THR 49 27.627 30.251 3.247 1.00 0.55 15G 389 ATOM 380 N THR 49 27.684 31.331 2.253 1.00 0.45 15G 389 ATOM 380 N THR 49 28.936 31.166 1.589 1.00 0.55 15G 391 ATOM 390 CB THR 49 27.669 31.331 2.255 1.00 0.55 15G 393 ATOM 390 CB THR 49 27.629 32.679 2.968 1.00 0.55 15G 393 ATOM 390 CB THR 49 28.936 31.166 1.589 1.00 0.55 15G 393 ATOM 390 CB THR 49 28.482 30.361 4.310 1.00 0.55 15G 393 ATOM 390 CB THR 49 28.482 30.361 4.310 1.00 0.55 15G 393 ATOM 390 CB THR 49 28.482 30.361 4.310 1.00 0.55 15G 393 ATOM 390 CB THR 49 28.482 30.361 4.310 1.00 0.55 15G 393 ATOM 390 CB THR 49 28.482 30.361 4.310 1.00 0.55 15G 393 ATOM 390 CB THR 49 28.482 30.361 4.310 1.00 0.55 15G 393 ATOM 390 CB ATOM 590 CB ATOM								28.35	0 5.74	5 1.00		
ATOM 376 OBZ GLU 47 19.030 27.016 4.803 1.00 0.44 186 377 ATOM 378 O GLU 47 24.413 28.215 5.800 1.00 0.44 186 378 ATOM 379 N GLU 48 23.282 29.852 5.800 1.00 0.44 186 379 ATOM 379 N GLU 48 23.282 29.852 4.730 1.00 0.45 186 380 ATOM 381 CB GLU 48 23.284 30.775 2.465 1.00 0.45 186 381 ATOM 382 CB GLU 48 23.284 30.775 2.465 1.00 0.45 186 381 ATOM 383 CD GLU 48 23.798 31.140 2.929 1.00 0.45 186 383 ATOM 383 CD GLU 48 23.798 31.2140 2.929 1.00 0.45 186 383 ATOM 383 CD GLU 48 23.798 31.2140 2.929 1.00 0.45 186 383 ATOM 383 CD GLU 48 23.878 33.215 2.041 1.00 0.45 186 383 ATOM 385 OEZ GLU 48 23.878 33.215 2.041 1.00 0.45 186 383 ATOM 385 OEZ GLU 48 23.878 33.215 2.041 1.00 0.45 186 383 ATOM 385 OEZ GLU 48 23.487 33.215 2.041 1.00 0.45 186 383 ATOM 385 OEZ GLU 48 23.487 33.215 2.041 1.00 0.45 186 386 ATOM 387 O GLU 48 23.487 33.215 2.041 1.00 0.45 186 386 ATOM 387 O GLU 48 23.487 33.215 2.041 1.00 0.45 186 386 ATOM 389 CB THR 49 25.647 28.553 2.528 1.00 0.45 186 386 ATOM 390 CB THR 49 27.624 30.365 3.758 1.00 0.55 186 389 ATOM 393 CD THR 49 27.624 31.331 2.235 1.00 0.55 186 389 ATOM 393 CD THR 49 27.624 32.679 2.968 1.00 0.55 186 393 ATOM 393 CD THR 49 27.629 32.679 2.968 1.00 0.55 186 393 ATOM 393 CD THR 49 28.482 30.361 1.06 1.05 91.00 0.55 186 393 ATOM 395 CB ATOM 397 CB ASN 50 31.925 28.990 4.291 1.00 0.44 186 396 ATOM 399 CD ASN 50 31.393 7.00 90 3.881 1.00 0.55 186 395 ATOM 399 CD ASN 50 31.393 7.00 90 3.881 1.00 0.44 186 396 ATOM 399 CD ASN 50 31.393 7.00 90 3.881 1.00 0.44 186 396 ATOM 400 ND2 ASN 50 31.346 27.765 1.7747 1.00 0.44 186 396 ATOM 400 ND2 ASN 50 31.346 27.765 1.7747 1.00 0.44 186 397 ATOM 400 ND2 ASN 50 31.346 27.784 1.00 0.25 186 400 ATOM 400 ND2 ASN 50 31.648 31.407 4.437 1.00 0.25 186 401 ATOM 400 ND2 ASN 50 31.383 32.472 4.355 1.00 0.25 186 401 ATOM 400 ND2 ASN 50 31.648 31.407 4.437 1.00 0.25 186 401 ATOM 400 ND2 ASN 50 31.648 31.407 4.437 1.00 0.25 186 401 ATOM 400 ND2 ASN 50 31.384 3.329 9.00 31.325 4.329 1.00 0.25 186 401 ATOM 400 ND2 ASN 50 31.383 33.383 30.109 4.291 1.00 0.44 186 411 ATOM 4	25	ATOM	375	OE1	GLU							1SG 375
ATCM 378 0 GLU 47 23.552 29.092 5.800 1.00 0.44 1SG 379 ATCM 379 N GLU 48 23.288 29.658 4.730 1.00 0.44 1SG 379 ATCM 380 CA GLU 48 23.741 29.655 3.387 1.00 0.45 1SG 380 ATCM 381 CB GLU 48 23.741 29.655 3.387 1.00 0.45 1SG 380 ATCM 382 CG GLU 48 23.788 32.140 2.929 1.00 0.45 1SG 381 ATCM 383 CD GLU 48 23.788 32.140 2.929 1.00 0.45 1SG 382 ATCM 385 OEZ GLU 48 23.788 32.140 2.929 1.00 0.45 1SG 383 ATCM 385 OEZ GLU 48 23.484 30.775 2.041 1.00 0.45 1SG 383 ATCM 386 C GLU 48 23.484 32.852 1.094 1.00 0.45 1SG 383 ATCM 387 O GLU 48 25.266 29.496 3.195 1.00 0.45 1SG 386 ATCM 388 N THR 49 26.087 30.365 3.758 1.00 0.45 1SG 386 ATCM 389 CA THR 49 27.664 31.331 2.235 1.00 0.45 1SG 388 ATCM 391 OGI THR 49 26.087 30.365 3.758 1.00 0.55 1SG 389 ATCM 393 C THR 49 27.664 31.331 2.235 1.00 0.55 1SG 389 ATCM 393 C THR 49 27.664 31.331 2.235 1.00 0.55 1SG 389 ATCM 393 C THR 49 27.664 31.331 2.235 1.00 0.55 1SG 389 ATCM 393 C THR 49 27.629 32.679 2.968 1.00 0.55 1SG 389 ATCM 393 C THR 49 27.629 32.679 2.968 1.00 0.55 1SG 393 ATCM 394 O THR 49 28.482 30.361 4.310 1.00 0.55 1SG 393 ATCM 395 CA ASN 50 31.925 28.990 4.291 1.00 0.44 1SG 396 ATCM 397 CB ASN 50 31.925 28.990 4.291 1.00 0.44 1SG 396 ATCM 398 C G ASN 50 31.925 28.990 4.291 1.00 0.44 1SG 396 ATCM 398 C G ASN 50 31.925 28.990 31.325 4.791 1.00 0.44 1SG 396 ATCM 400 ND2 ASN 50 31.044 27.481 5.927 1.00 0.44 1SG 397 ATCM 400 ND2 ASN 50 31.648 31.407 4.437 1.00 0.44 1SG 396 ATCM 401 C ASR 50 31.044 27.481 5.927 1.00 0.44 1SG 402 ATCM 404 CA SER 51 33.384 32.473 4.237 1.00 0.25 1SG 404 ATCM 406 CG SER 51 33.383 34.545 3.215 1.00 0.25 1SG 407 ATCM 407 C SER 51 33.383 34.545 3.215 1.00 0.14 1SG 411 ATCM 410 CA SER 52 31.35 3.30 3.30 3.575 0.00 0.14 1SG 411 ATCM 410 CB SER 52 31.35 3.30 3.388 3.575 0.027 1.00 0.14 1SG 411 ATCM 417 CB SER 52 31.35 3.30 3.30 3.30 3.00 0.00 0.14 1SG 411 ATCM 410 CB SER 52 31.30 3.30 3.30 3.30 3.00 0.00 0.14 1SG 411 ATCM 410 CB SER 52 31.30 3.30 3.30 3.30 3.00 0.00 0.14 1SG 411 ATCM 410 CB SER 52 31.30 3.30 3.30 3.30 0.00 0.00 0.14 1SG 411 ATCM 410 CB SER	25						19.030	27.01	6 4.80			
379 N GLU 48 23.288 29.888 1.00 1.00 0.45 15G 389 389 381 380 CA GUU 48 23.244 29.635 3.387 1.00 0.45 15G 380 ATOM 381 CB GLU 48 23.244 32.245 1.00 0.45 15G 381 381 381 381 385 0E2 GLU 48 23.244 32.882 1.00 0.45 15G 382 383 384 385 0E2 GLU 48 23.187 33.215 2.041 1.00 0.45 15G 382 384 387 385 0E2 GLU 48 23.187 33.215 2.041 1.00 0.45 15G 382 384 387 385 0E2 GLU 48 22.440 32.852 1.094 1.00 0.45 15G 382 384 387 385 0E2 GLU 48 25.266 29.496 3.195 1.00 0.45 15G 382 386 387 387 0.00 387 0.00 6.14 48 25.667 28.553 2.528 1.00 0.45 15G 385 386 387 387 0.00 387 0.00 6.14 48 25.667 28.553 2.528 1.00 0.45 15G 385 386 387 387 0.00 387 0.00 388 N THR 49 26.087 30.365 3.758 1.00 0.45 15G 388 380 387 387 0.00 389 CA THR 49 27.427 30.251 3.247 1.00 0.55 15G 389 380 387 0.00 389 CA THR 49 27.684 31.331 2.235 1.00 0.55 15G 389 380 387 0.00 389 CA THR 49 28.936 31.166 1.589 1.00 0.55 15G 389 380 380 380 380 380 380 380 380 380 380									_		0.44	1SG 378
ATOM 381 CB GIU 48 23.741 29.635 3.387 1.00 0.45 15G 381 15G 381 15G 382 387 383 CD GIU 48 23.788 30.775 2.465 1.00 0.45 15G 382 382 387 383 CD GIU 48 23.788 32.140 2.929 1.00 0.45 15G 383 382 387 385					GLU	48	23.288	29.85			-	
ATOM 382 CG GIU 48 23.187 32.140 2.929 1.00 0.45 1SG 382 ATOM 383 CD GIU 48 23.187 33.215 2.041 1.00 0.45 1SG 383 ATOM 385 CE2 GIU 48 22.440 32.852 1.094 1.00 0.45 1SG 383 385 ATOM 386 C GIU 48 25.264 29.496 3.195 1.00 0.45 1SG 386 ATOM 386 C GIU 48 25.266 29.496 3.195 1.00 0.45 1SG 386 ATOM 387 O GIU 48 25.266 29.496 3.195 1.00 0.45 1SG 386 ATOM 388 N THR 49 25.2647 28.553 3.758 1.00 0.45 1SG 387 ATOM 389 CB THR 49 27.427 30.251 3.247 1.00 0.55 1SG 389 ATOM 389 CB THR 49 27.427 30.251 3.247 1.00 0.55 1SG 389 ATOM 390 CB THR 49 27.427 30.251 3.247 1.00 0.55 1SG 389 ATOM 391 CGI THR 49 28.936 31.166 1.589 1.00 0.55 1SG 391 ATOM 393 C THR 49 27.427 30.251 3.247 1.00 0.55 1SG 393 ATOM 393 C THR 49 27.427 30.251 3.247 1.00 0.55 1SG 393 ATOM 393 C THR 49 27.427 30.251 3.247 1.00 0.55 1SG 393 ATOM 393 C THR 49 27.427 30.251 3.247 1.00 0.55 1SG 393 ATOM 393 C THR 49 27.427 30.251 3.247 1.00 0.55 1SG 393 ATOM 393 C THR 49 27.427 30.251 3.247 1.00 0.55 1SG 393 ATOM 393 C ASN 50 30.937 30.109 4.655 1.00 0.55 1SG 393 ATOM 394 C ASN 50 30.937 30.109 4.655 1.00 0.44 1SG 396 ATOM 395 N ASN 50 29.736 30.090 3.881 1.00 0.44 1SG 397 ATOM 396 CG ASN 50 31.352 7.665 4.747 1.00 0.44 1SG 397 ATOM 399 CDI ASN 50 31.325 7.665 4.747 1.00 0.44 1SG 398 ATOM 400 ND2 ASN 50 31.352 7.665 4.747 1.00 0.44 1SG 399 ATOM 400 ND2 ASN 50 31.044 27.481 5.927 1.00 0.44 1SG 401 ATOM 402 O ASN 50 31.038 32.472 4.355 1.00 0.25 1SG 404 ATOM 404 CA SER 51 33.843 32.473 4.237 1.00 0.25 1SG 405 ATOM 407 C SER 51 33.843 32.473 4.237 1.00 0.25 1SG 406 ATOM 407 C SER 51 33.3455 33.328 3.073 1.00 0.25 1SG 407 ATOM 408 N SER 52 33.3750 33.288 -0.481 1.00 0.14 1SG 411 ATOM 412 CG SER 52 31.035 32.290 4.049 1.00 0.25 1SG 407 ATOM 413 C SER 52 33.3750 33.288 -0.481 1.00 0.14 1SG 411 ATOM 412 CG SER 52 33.3750 33.288 -0.481 1.00 0.14 1SG 411 ATOM 413 C SER 52 31.035 32.204 0.274 1.00 0.14 1SG 411 ATOM 418 CG LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 412 ATOM 419 CG LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 412 ATOM 419 CG LEU 53 29.346 34.291 -0.00 0.99 1SG 420 AT	30								3.38	7 1.00	0.45	
ATOM 384 OB GLU 48 23.487 33.215 2.041 1.00 0.45 18G 3884 384 OB GLU 48 22.440 32.852 1.094 1.00 0.45 18G 3885 3864 32.840 32.852 1.094 1.00 0.45 18G 3885 3864 32.460 32.852 1.094 1.00 0.45 18G 3885 3.400 32.852 3.400 3.		MOTA	382	CG	GLU							
35 ATOM 385 OE2 GIU 48 23.459 34.417 2.302 1.00 0.45 1SG 385 ATOM 386 C GJU 48 25.626 29.496 31.95 1.00 0.45 1SG 386 ATOM 387 O GIU 48 25.647 28.553 2.528 1.00 0.45 1SG 387 ATOM 389 CA THR 49 26.087 30.365 3.758 1.00 0.45 1SG 388 ATOM 389 CA THR 49 27.427 30.251 3.247 1.00 0.55 1SG 389 ATOM 391 OGI THR 49 27.629 32.679 2.968 1.00 0.55 1SG 399 ATOM 392 CG THR 49 27.629 32.679 2.968 1.00 0.55 1SG 391 ATOM 392 CG THR 49 28.936 31.166 1.589 1.00 0.55 1SG 392 ATOM 393 C THR 49 28.482 30.361 4.310 1.00 0.55 1SG 392 ATOM 393 C THR 49 28.482 30.361 4.310 1.00 0.55 1SG 393 ATOM 394 O THR 49 28.482 30.361 4.310 1.00 0.55 1SG 393 ATOM 394 O THR 49 28.213 30.658 5.473 1.00 0.55 1SG 393 ATOM 396 CA ASN 50 30.937 30.109 4.665 1.00 0.44 1SG 396 ATOM 397 CB ASN 50 31.925 28.990 4.291 1.00 0.44 1SG 397 ATOM 398 CG ASN 50 31.935 28.990 4.291 1.00 0.44 1SG 397 ATOM 399 ODI ASN 50 31.044 27.481 5.927 1.00 0.44 1SG 399 ATOM 399 ODI ASN 50 31.044 27.481 5.927 1.00 0.44 1SG 399 ATOM 399 ODI ASN 50 31.044 27.481 5.927 1.00 0.44 1SG 400 ATOM 400 ND2 ASN 50 31.048 27.481 5.927 1.00 0.44 1SG 400 ATOM 400 ND2 ASN 50 31.688 31.407 4.437 1.00 0.44 1SG 400 ATOM 400 ND2 ASN 50 31.048 31.407 4.437 1.00 0.44 1SG 400 ATOM 404 CA SSR 51 32.990 31.325 4.329 1.00 0.25 1SG 404 ATOM 404 CA SSR 51 33.843 32.473 4.325 1.00 0.25 1SG 405 ATOM 406 CG SER 51 35.323 32.473 4.227 1.00 0.25 1SG 405 ATOM 407 C SER 51 35.323 32.473 4.237 1.00 0.25 1SG 405 ATOM 408 CS SER 52 33.384 32.473 4.237 1.00 0.25 1SG 405 ATOM 408 CS SER 52 33.383 34.545 3.215 1.00 0.25 1SG 405 ATOM 410 CA SER 52 33.383 32.473 4.227 1.00 0.25 1SG 405 ATOM 410 CB SER 52 33.383 32.473 4.227 1.00 0.25 1SG 405 ATOM 410 CB SER 52 33.383 32.473 4.227 1.00 0.25 1SG 405 ATOM 410 CB SER 52 33.383 32.473 4.227 1.00 0.14 1SG 411 1SG 411 ATOM 410 CB SER 52 33.383 32.473 4.227 1.00 0.14 1SG 411 ATOM 410 CB SER 52 33.388 -0.481 1.00 0.09 1SG 411 ATOM 410 CB SER 52 33.388 -0.481 1.00 0.09 1SG 411 ATOM 410 CB SER 52 33.488 0.888 0.886 1.00 0.09 1SG 412 ATOM 411 CB SER 52 31.480 33.383 0.406 1.00 0.09 1SG								33.215	2.04	1.00		
ATOM 386 C GLU 48 25.226 29.496 3.195 1.00 0.45 1SG 387 ATOM 388 N THR 49 26.087 30.365 3.758 1.00 0.45 1SG 388 ATOM 389 CA THR 49 26.087 30.365 3.758 1.00 0.45 1SG 388 ATOM 390 CB THR 49 27.629 30.365 3.758 1.00 0.55 1SG 399 ATOM 391 OG1 THR 49 27.629 31.166 1.589 1.00 0.55 1SG 391 ATOM 392 CG2 THR 49 27.629 32.679 2.968 1.00 0.55 1SG 391 ATOM 393 C THR 49 28.936 31.166 1.589 1.00 0.55 1SG 392 ATOM 394 O THR 49 28.482 30.361 4.310 0.55 1SG 393 ATOM 395 N ASN 50 29.736 30.090 3.881 1.00 0.55 1SG 393 ATOM 395 N ASN 50 29.736 30.090 3.881 1.00 0.55 1SG 395 ATOM 397 CB ASN 50 31.925 28.990 4.291 1.00 0.44 1SG 396 ATOM 398 CG ASN 50 31.353 27.665 4.747 1.00 0.44 1SG 398 ATOM 398 CG ASN 50 31.353 27.665 4.747 1.00 0.44 1SG 398 ATOM 399 ND1 ASN 50 31.925 28.990 4.291 1.00 0.44 1SG 398 ATOM 399 ND2 ASN 50 31.353 27.665 4.747 1.00 0.44 1SG 398 ATOM 400 ND2 ASN 50 31.353 27.665 4.747 1.00 0.44 1SG 398 ATOM 400 ND2 ASN 50 31.353 27.665 4.747 1.00 0.44 1SG 400 ATOM 403 N SER 51 33.883 27.665 4.747 1.00 0.44 1SG 400 ATOM 404 ND ND2 ASN 50 31.638 32.472 4.355 1.00 0.44 1SG 401 ATOM 403 N SER 51 33.883 32.473 4.337 1.00 0.25 1SG 404 ATOM 404 ND ND2 ASN 50 31.638 32.473 4.355 1.00 0.44 1SG 403 ATOM 405 CB SER 51 33.883 32.473 4.237 1.00 0.25 1SG 404 ATOM 409 N SER 51 33.883 32.473 4.237 1.00 0.25 1SG 405 ATOM 409 N SER 52 33.338 34.545 3.225 1.00 0.44 1SG 401 ATOM 409 N SER 52 33.338 34.545 3.225 1.00 0.14 1SG 411 1SG 411 ATOM 412 CG SER 52 33.334 32.473 4.237 1.00 0.25 1SG 408 ATOM 409 N SER 52 33.338 34.545 3.225 1.00 0.14 1SG 411 1SG 411 ATOM 412 CG SER 52 33.334 32.473 1.887 1.00 0.14 1SG 411 ATOM 412 CG SER 52 33.334 32.473 1.887 1.00 0.14 1SG 411 ATOM 412 CG SER 52 33.334 32.473 1.887 1.00 0.14 1SG 411 ATOM 412 CG SER 52 33.334 32.473 1.00 0.09 1SG 419 ATOM 419 CD2 LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 419 ATOM 410 CD SER 52 31.035 32.204 0.274 1.00 0.14 1SG 411 ATOM 412 CG LEU 53 29.346 34.696 0.368 1.00 0.09 1SG 419 ATOM 410 CD LEU 53 29.346 34.696 0.368 1.00 0.09 1SG 419 ATOM 410 CD LEU 53 29.346 34.696 0.368 1.0	3.5	MOTA										1SG 385
ATOM 388 N THR 49 26.647 30.365 3.750 1.00 0.45 18G 388 ATOM 389 CA THR 49 27.427 30.251 3.247 1.00 0.55 18G 390 ATOM 390 CB THR 49 27.668 31.331 2.235 1.00 0.55 18G 391 ATOM 392 CG2 THR 49 27.629 32.679 2.968 1.00 0.55 18G 393 ATOM 393 C THR 49 28.842 30.361 4.310 1.00 0.55 18G 393 ATOM 393 C THR 49 28.842 30.361 4.310 1.00 0.55 18G 393 ATOM 394 C THR 49 28.842 30.361 4.310 1.00 0.55 18G 393 ATOM 395 N ASN 50 29.736 30.090 3.881 1.00 0.55 18G 393 ATOM 395 CA ASN 50 30.937 30.109 4.665 1.00 0.44 18G 396 ATOM 399 CD ASN 50 31.925 28.990 4.291 1.00 0.44 18G 397 ATOM 399 CD ASN 50 31.335 27.665 4.73 1.00 0.44 18G 399 ATOM 399 CD ASN 50 31.335 27.665 4.747 1.00 0.44 18G 399 ATOM 399 CD ASN 50 31.036 32.6715 3.790 1.00 0.44 18G 399 ATOM 399 CD ASN 50 31.036 32.472 4.355 1.00 0.44 18G 400 ATOM 401 C ASN 50 31.038 32.472 4.355 1.00 0.44 18G 400 ATOM 402 C ASN 50 31.038 32.472 4.355 1.00 0.44 18G 400 ATOM 403 N SER 51 32.990 31.325 4.329 1.00 0.25 18G 404 ATOM 406 CB SER 51 33.843 32.473 4.237 1.00 0.25 18G 405 ATOM 407 C SER 51 33.843 32.473 4.237 1.00 0.25 18G 406 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 406 ATOM 409 N SER 52 33.234 32.733 1.887 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 18G 407 ATOM 408 C SER 52 31.035 33.288 0.481 1.00 0.014 18G 411 18G 412 ATOM 415 C SER 52 31.685 33.595 1.259 1.00 0.09 18G 417 ATOM 415 C	35						25.226	29.496	3.195	1.00		
ATOM 389 CA THR 49 27.427 30.251 3.247 1.00 0.55 1SG 389 ATOM 390 CB THR 49 27.624 31.331 2.235 1.00 0.55 1SG 390 ATOM 391 OG1 THR 49 27.629 32.679 2.968 1.00 0.55 1SG 392 ATOM 393 C THR 49 28.482 30.361 4.310 1.00 0.55 1SG 393 ATOM 394 O THR 49 28.482 30.361 4.310 1.00 0.55 1SG 393 ATOM 395 N ASN 50 29.736 30.090 3.881 1.00 0.55 1SG 394 ATOM 396 CA ASN 50 31.925 28.990 4.291 1.00 0.44 1SG 396 ATOM 397 CB ASN 50 31.925 28.990 4.291 1.00 0.44 1SG 397 ATOM 399 OD1 ASN 50 31.335 27.665 4.747 1.00 0.44 1SG 398 ATOM 399 OD1 ASN 50 31.153 26.715 3.790 1.00 0.44 1SG 400 ATOM 401 C ASN 50 31.648 31.407 4.437 1.00 0.44 1SG 400 ATOM 402 O ASN 50 31.038 32.472 4.355 1.00 0.44 1SG 403 ATOM 404 CA SER 51 32.990 31.325 4.329 1.00 0.25 1SG 405 ATOM 405 CB SER 51 35.506 31.465 2.792 1.00 0.25 1SG 405 ATOM 407 C SER 51 33.338 32.473 4.237 1.00 0.25 1SG 406 ATOM 408 O SER 52 33.338 32.473 4.237 1.00 0.25 1SG 406 ATOM 409 N SER 52 33.234 32.733 1.887 1.00 0.25 1SG 406 ATOM 401 CA SER 52 33.234 32.733 1.887 1.00 0.25 1SG 406 ATOM 407 C SER 51 33.338 34.545 33.215 1.00 0.25 1SG 406 ATOM 408 O SER 52 33.338 34.545 3.215 1.00 0.25 1SG 406 ATOM 401 CA SER 52 33.234 32.733 1.887 1.00 0.14 1SG 411 ATOM 410 CA SER 52 33.750 33.288 -0.481 1.00 0.14 1SG 411 ATOM 410 CA SER 52 33.750 33.288 -0.481 1.00 0.14 1SG 411 ATOM 410 CA SER 52 33.750 33.288 -0.481 1.00 0.14 1SG 411 ATOM 410 CB SER 52 31.480 33.343 0.406 1.00 0.09 1SG 412 ATOM 410 CB LEU 53 28.319 34.487 0.251 1.00 0.09 1SG 417 ATOM 410 CB LEU 53 26.482 33.208 0.368 1.00 0.09 1SG 419 ATOM 410 CB LEU 53 26.482 33.208 0.368 1.00 0.09 1SG 419 ATOM 410 CB LEU 53 26.482 33.208 0.369 1.00 0.09 1SG 420 ATOM 410 CB LEU 53 26.482 33.208 0.369 1.00 0.09 1SG 421											0.45	1SG 388
40 ATCM 391 OG1 THR 49 27.684 31.331 2.235 1.00 0.55 1SG 391 ATCM 392 CG2 THR 49 27.629 32.679 2.968 1.00 0.55 1SG 392 ATCM 393 C THR 49 28.482 30.361 4.310 1.00 0.55 1SG 393 ATCM 394 O THR 49 28.482 30.361 4.310 1.00 0.55 1SG 394 ATCM 395 N ASN 50 29.736 30.090 3.881 1.00 0.55 1SG 395 ATCM 396 CA ASN 50 30.937 30.109 4.665 1.00 0.44 1SG 396 ATCM 397 CB ASN 50 31.335 27.665 4.747 1.00 0.44 1SG 397 ATCM 399 OD1 ASN 50 31.335 27.665 4.747 1.00 0.44 1SG 398 ATCM 399 OD1 ASN 50 31.335 27.665 4.747 1.00 0.44 1SG 398 ATCM 399 OD1 ASN 50 31.648 31.407 4.437 1.00 0.44 1SG 400 ATCM 400 ND2 ASN 50 31.648 31.407 4.437 1.00 0.44 1SG 401 ATCM 402 O ASN 50 31.038 32.472 4.355 1.00 0.44 1SG 402 ATCM 403 N SER 51 32.990 31.325 4.329 1.00 0.25 1SG 404 ATCM 404 CA SER 51 33.843 32.473 4.237 1.00 0.25 1SG 405 ATCM 406 OG SER 51 35.323 32.099 4.049 1.00 0.25 1SG 406 ATCM 407 C SER 51 33.345 33.345 32.473 4.237 1.00 0.25 1SG 406 ATCM 409 N SER 52 33.338 34.545 3.215 1.00 0.25 1SG 408 ATCM 409 N SER 52 33.338 34.545 3.215 1.00 0.25 1SG 408 ATCM 409 N SER 52 33.234 32.733 1.887 1.00 0.25 1SG 408 ATCM 409 N SER 52 33.338 34.545 3.215 1.00 0.25 1SG 408 ATCM 410 CA SER 51 33.338 34.545 3.215 1.00 0.25 1SG 408 ATCM 410 CA SER 52 32.906 33.575 0.772 1.00 0.14 1SG 411 ATCM 411 CB SER 52 31.480 33.348 -0.481 1.00 0.14 1SG 411 ATCM 412 OG SER 52 31.480 33.345 30.496 1.00 0.25 1SG 408 ATCM 413 C SER 52 31.480 33.345 30.496 1.00 0.09 1SG 416 ATCM 416 CA LEU 53 29.906 33.575 0.772 1.00 0.14 1SG 411 ATCM 416 CA LEU 53 29.906 33.575 0.772 1.00 0.14 1SG 411 ATCM 416 CA LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 416 ATCM 417 CB LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 417 ATCM 420 CD1 LEU 53 26.482 33.208 0.368 1.00 0.09 1SG 419 ATCM 420 CD1 LEU 53 26.482 33.208 0.368 1.00 0.09 1SG 412 ATCM 420 CD1 LEU 53 26.482 33.208 0.368 1.00 0.09 1SG 422 ATCM 422 0 CD1 LEU 53 26.482 33.208 0.368 1.00 0.09 1SG 422 ATCM 422 0 CD1 LEU 53 26.482 33.208 0.298 1.00 0.09 1SG 422 ATCM 422 0 CD1 LEU 53 26.482 33.208 0.298 1.00 0.09 1SG 422						49	27.427	30.251	3.247			
ATOM 392 CG2 THR 49 27.629 32.679 2.968 1.00 0.55 1SG 393 ATOM 393 C THR 49 28.482 30.361 4.310 1.00 0.55 1SG 393 ATOM 395 N ASN 50 29.736 30.090 3.881 1.00 0.55 1SG 395 ATOM 396 CA ASN 50 30.937 30.109 4.665 1.00 0.44 1SG 396 ATOM 397 CB ASN 50 31.925 28.990 4.291 1.00 0.44 1SG 397 ATOM 398 CG ASN 50 31.335 27.665 4.747 1.00 0.44 1SG 399 ATOM 399 OD1 ASN 50 31.335 27.665 4.747 1.00 0.44 1SG 399 ATOM 400 ND2 ASN 50 31.648 31.407 4.371 1.00 0.44 1SG 400 ATOM 401 C ASN 50 31.648 31.407 4.371 1.00 0.44 1SG 401 ATOM 402 O ASN 50 31.648 31.407 4.371 1.00 0.44 1SG 403 ATOM 403 N SER 51 32.990 31.325 4.329 1.00 0.25 1SG 406 ATOM 404 CA SER 51 33.843 32.473 4.237 1.00 0.25 1SG 406 ATOM 407 C SER 51 33.843 32.473 4.237 1.00 0.25 1SG 406 ATOM 407 C SER 51 33.384 32.473 4.237 1.00 0.25 1SG 406 ATOM 407 C SER 51 33.345 33.288 3.073 1.00 0.25 1SG 409 ATOM 408 O SER 51 33.338 34.545 3.215 1.00 0.25 1SG 409 ATOM 409 N SER 52 33.234 32.733 1.887 1.00 0.25 1SG 409 ATOM 410 CA SER 52 33.234 32.733 1.887 1.00 0.25 1SG 409 ATOM 411 CB SER 52 33.355 33.328 3.073 1.00 0.25 1SG 409 ATOM 410 CA SER 52 33.355 33.328 3.073 1.00 0.25 1SG 409 ATOM 410 CA SER 52 33.355 33.328 3.073 1.00 0.25 1SG 409 ATOM 410 CA SER 52 33.356 33.288 0.073 1.00 0.14 1SG 411 ATOM 412 OG SER 52 33.750 33.288 0.481 1.00 0.14 1SG 411 ATOM 413 C SER 52 33.750 33.288 0.481 1.00 0.14 1SG 412 ATOM 415 N LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 415 ATOM 416 CA LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 415 ATOM 417 CB LEU 53 26.856 34.696 0.368 1.00 0.09 1SG 416 ATOM 417 CB LEU 53 26.856 34.696 0.368 1.00 0.09 1SG 419 ATOM 420 CD1 LEU 53 26.856 34.696 0.368 1.00 0.09 1SG 421 ATOM 420 CD1 LEU 53 26.856 34.696 0.368 1.00 0.09 1SG 421 ATOM 420 CD1 LEU 53 26.856 34.696 0.368 1.00 0.09 1SG 421 ATOM 421 C LEU 53 29.195 34.941 -1.473 1.00 0.09 1SG 422	40									1.00	0.55	1SG 391
ATOM 394 C THR 49 28.482 30.361 4.310 1.00 0.55 1SG 394 ATOM 395 N ASN 50 29.736 30.658 5.473 1.00 0.55 1SG 395 ATOM 396 CA ASN 50 30.937 30.109 4.665 1.00 0.44 1SG 396 ATOM 397 CB ASN 50 31.925 28.990 4.291 1.00 0.44 1SG 397 ATOM 399 OD1 ASN 50 31.335 27.665 4.747 1.00 0.44 1SG 399 ATOM 399 OD1 ASN 50 31.153 26.715 3.790 1.00 0.44 1SG 400 ATOM 400 ND2 ASN 50 31.648 31.407 4.437 1.00 0.44 1SG 401 ATOM 403 N SER 51 32.990 31.325 4.329 1.00 0.44 1SG 402 ATOM 403 N SER 51 33.843 32.472 4.355 1.00 0.44 1SG 403 ATOM 404 CA SER 51 33.843 32.473 4.237 1.00 0.25 1SG 406 ATOM 406 OG SER 51 33.5506 31.465 2.792 1.00 0.25 1SG 406 ATOM 407 C SER 51 33.338 34.545 3.215 1.00 0.25 1SG 408 ATOM 409 N SER 52 33.234 32.33 1.887 1.00 0.25 1SG 408 ATOM 409 N SER 52 33.234 32.33 1.887 1.00 0.25 1SG 408 ATOM 410 CA SER 52 33.234 32.33 1.887 1.00 0.25 1SG 408 ATOM 410 CA SER 52 33.234 32.33 1.887 1.00 0.25 1SG 408 ATOM 410 CA SER 52 33.234 32.33 1.887 1.00 0.25 1SG 408 ATOM 410 CA SER 52 33.234 32.33 1.887 1.00 0.25 1SG 408 ATOM 410 CA SER 52 33.234 32.733 1.00 0.25 1SG 408 ATOM 410 CA SER 52 33.358 33.328 3.073 1.00 0.25 1SG 408 ATOM 410 CA SER 52 33.358 33.328 3.073 1.00 0.25 1SG 408 ATOM 410 CA SER 52 33.358 33.328 3.073 1.00 0.25 1SG 408 ATOM 410 CA SER 52 33.358 34.545 3.215 1.00 0.14 1SG 411 ATOM 412 OG SER 52 33.750 33.288 -0.481 1.00 0.14 1SG 411 ATOM 413 C SER 52 33.070 34.437 0.251 1.00 0.14 1SG 413 ATOM 414 O SER 52 31.035 32.204 0.274 1.00 0.14 1SG 413 ATOM 415 N LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 416 ATOM 419 CD2 LEU 53 28.319 34.889 0.816 1.00 0.09 1SG 416 ATOM 419 CD2 LEU 53 28.319 34.899 0.816 1.00 0.09 1SG 419 ATOM 420 CD1 LEU 53 28.819 34.947 -1.1473 1.00 0.09 1SG 420 ATOM 420 O LEU 53 29.195 34.941 -1.473 1.00 0.09 1SG 422				CG2	THR	49						
45 ATOM 395 N ASN 50 29.736 30.090 3.881 1.00 0.44 1SG 395 ATOM 397 CB ASN 50 30.937 30.109 4.665 1.00 0.44 1SG 397 ATOM 398 CG ASN 50 31.925 28.990 4.291 1.00 0.44 1SG 398 ATOM 399 OD1 ASN 50 31.044 27.481 5.927 1.00 0.44 1SG 399 ATOM 400 ND2 ASN 50 31.044 27.481 5.927 1.00 0.44 1SG 400 ATOM 401 C ASN 50 31.648 31.407 4.437 1.00 0.44 1SG 401 ATOM 403 N SER 51 32.990 31.325 4.329 1.00 0.44 1SG 403 ATOM 403 N SER 51 32.990 31.325 4.329 1.00 0.25 1SG 404 ATOM 405 CB SER 51 35.323 32.099 4.049 1.00 0.25 1SG 406 ATOM 406 OG SER 51 35.323 32.099 4.049 1.00 0.25 1SG 406 ATOM 406 OG SER 51 33.455 33.328 3.073 1.00 0.25 1SG 406 ATOM 400 N SER 52 33.338 34.545 32.15 1.00 0.25 1SG 408 ATOM 400 CA SER 51 33.338 34.545 32.15 1.00 0.25 1SG 408 ATOM 400 CA SER 52 33.234 32.333 1.887 1.00 0.25 1SG 408 ATOM 401 CA SER 52 33.234 32.333 1.887 1.00 0.25 1SG 408 ATOM 401 CA SER 52 33.234 32.333 1.887 1.00 0.25 1SG 408 ATOM 401 CA SER 52 33.234 32.333 1.887 1.00 0.25 1SG 408 ATOM 410 CA SER 52 33.356 33.575 0.772 1.00 0.25 1SG 409 ATOM 410 CA SER 52 33.234 32.333 1.887 1.00 0.14 1SG 411 ATOM 412 OG SER 52 33.750 33.288 -0.481 1.00 0.14 1SG 411 ATOM 413 C SER 52 31.035 32.204 0.274 1.00 0.14 1SG 411 ATOM 414 O SER 52 31.480 33.334 0.406 1.00 0.14 1SG 411 ATOM 414 O SER 52 31.480 33.334 0.406 1.00 0.14 1SG 413 ATOM 414 O SER 52 31.480 33.335 0.406 1.00 0.14 1SG 413 ATOM 414 O SER 52 31.480 33.335 0.406 1.00 0.09 1SG 418 ATOM 417 CB LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 418 ATOM 419 CD2 LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 418 ATOM 419 CD2 LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 418 ATOM 420 CD1 LEU 53 26.482 33.208 0.298 1.00 0.09 1SG 419 ATOM 420 CD1 LEU 53 26.482 33.208 0.298 1.00 0.09 1SG 422 ATOM 421 C LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 412 ATOM 422 O LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 422 ATOM 422 O LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 422 ATOM 422 O LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 422 ATOM 422 O LEU 53 29.476 36.283 34.271 -0.250 1.00 0.09 1SG 422 ATOM 422 O LEU 53 26.482 33.208 0.298 1.0									4.310	1.00	0.55	
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ATOM 415 N LEU 53 30.709 34.437 0.251 1.00 0.14 1SG 415 ATOM 416 CA LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 416 ATOM 417 CB LEU 53 28.319 34.889 0.816 1.00 0.09 1SG 417 ATOM 418 CG LEU 53 26.856 34.696 0.368 1.00 0.09 1SG 419 ATOM 419 CD2 LEU 53 25.893 35.495 1.259 1.00 0.09 1SG 419 ATOM 420 CD1 LEU 53 26.482 33.208 0.298 1.00 0.09 1SG 420 ATOM 421 C LEU 53 29.195 34.941 -1.473 1.00 0.09 1SG 421 ATOM 422 0 LEU 53 29.476 36.130 1.00 0.09 1SG 422									0.406	1.00	0.14	1SG 414
ATOM 416 CA LEU 53 29.346 34.271 -0.150 1.00 0.09 1SG 417 ATOM 417 CB LEU 53 28.319 34.889 0.816 1.00 0.09 1SG 418 ATOM 418 CG LEU 53 26.856 34.696 0.368 1.00 0.09 1SG 419 ATOM 419 CD2 LEU 53 25.893 35.495 1.259 1.00 0.09 1SG 420 ATOM 420 CD1 LEU 53 26.482 33.208 0.298 1.00 0.09 1SG 420 ATOM 421 C LEU 53 29.195 34.941 -1.473 1.00 0.09 1SG 422 ATOM 422 0 LEU 53 29.476 36.130 1.00 0.09 1SG 422	65	ATOM 4	115 N	I LE	EU 5:							
ATOM 418 CG LEU 53 26.856 34.696 0.368 1.00 0.09 1SG 418 ATOM 419 CD2 LEU 53 25.893 35.495 1.259 1.00 0.09 1SG 420 ATOM 420 CD1 LEU 53 26.482 33.208 0.298 1.00 0.09 1SG 420 ATOM 421 C LEU 53 29.195 34.941 -1.473 1.00 0.09 1SG 421 ATOM 422 0 LEU 53 29.476 36.130 1.00 0.09 1SG 422	03						29.346	34.271	-0.150	1.00		
ATOM 419 CD2 LEU 53 25.893 35.495 1.259 1.00 0.09 1SG 419 ATOM 420 CD1 LEU 53 26.482 33.208 0.298 1.00 0.09 1SG 420 ATOM 421 C LEU 53 29.195 34.941 -1.473 1.00 0.09 1SG 421 ATOM 422 0 LEU 53 29.476 36.130 1.00 0.09 1SG 422		ATOM 4	18 C	G LE	υ 5:							1SG 418
70 ATOM 421 C LEU 53 29.195 34.941 -1.473 1.00 0.09 1sG 421 ATOM 422 O LEU 53 29.476 36.130					T 53	3	25.893	35.495		_		
ATOM 422 O LEU 53 29 476 36 130 1.00 0.09 1SG 422	70	ATOM 4	21 C							1.00	0.09	1SG 421
		ATOM 4	22 o									

5	ATOM 423 N ASN 54 ATOM 424 CA ASN 54 ATOM 425 CB ASN 54 ATOM 426 CG ASN 54 ATOM 427 OD1 ASN 54 ATOM 428 ND2 ASN 54	28.584 34.749 -3.786 1.00 0.09 29.349 34.011 -4.897 1.00 0.09 29.234 34.837 -6.169 1.00 0.09 28.770 35.975 -6.145 1.00 0.09	1SG 424 1SG 425 1SG 426 1SG 427 1SG 428
10	ATOM 429 C ASN 54 ATOM 430 O ASN 54 ATOM 431 N ILE 55 ATOM 432 CA ILE 55 ATOM 433 CB ILE 55 ATOM 434 CG2 ILE 55	27.137 34.629 -4.118 1.00 0.09 26.544 33.562 -3.972 1.00 0.09 26.522 35.736 -4.566 1.00 0.08 25.141 35.665 -4.922 1.00 0.08 24.258 36.575 -4.120 1.00 0.08	1SG 429 1SG 430 1SG 431 1SG 432 1SG 433 1SG 434
15	ATOM 435 CG1 ILE 55 ATOM 436 CD1 ILE 55 ATOM 437 C ILE 55 ATOM 438 O ILE 55 ATOM 439 N VAL 56 ATOM 440 CA VAL 56	24.636 38.044 -4.369 1.00 0.08 23.600 39.030 -3.832 1.00 0.08 25.039 36.115 -6.337 1.00 0.08 25.773 36.998 -6.779 1.00 0.08 24.119 35.493 -7.090 1.00 0.10	1SG 435 1SG 436 1SG 437 1SG 438 1SG 439 1SG 440
20	ATOM 440 CA VAL 56 ATOM 441 CB VAL 56 ATOM 442 CG1 VAL 56 ATOM 443 CG2 VAL 56 ATOM 444 C VAL 56 ATOM 445 O VAL 56	23.922 35.858 -8.456 1.00 0.10 23.985 34.683 -9.389 1.00 0.10 23.615 35.140 -10.810 1.00 0.10 25.383 34.050 -9.280 1.00 0.10 22.544 36.412 -8.532 1.00 0.10	1SG 441 1SG 442 1SG 443 1SG 444 1SG 445
25	ATOM 446 N ASN 57 ATOM 447 CA ASN 57 ATOM 448 CB ASN 57 ATOM 449 CG ASN 57 ATOM 450 OD1 ASN 57	22.312 37.292 -9.523 1.00 0.11 21.035 37.906 -9.706 1.00 0.11 19.953 36.958 -10.250 1.00 0.11 18.801 37.822 -10.747 1.00 0.11 18.420 38.801 -10.107 1.00 0.11	1SG 446 1SG 447 1SG 448 1SG 449 1SG 450 1SG 451
30	ATOM 451 ND2 ASN 57 ATOM 452 C ASN 57 ATOM 453 O ASN 57 ATOM 454 N ALA 58 ATOM 455 CA ALA 58 ATOM 456 CB ALA 58	18.239 37.461 -11.932 1.00 0.11 20.576 38.473 -8.404 1.00 0.11 19.548 38.066 -7.865 1.00 0.11 21.353 39.425 -7.850 1.00 0.21 20.945 40.022 -6.615 1.00 0.21	1SG 452 1SG 453 1SG 454 1SG 455 1SG 456
35	ATOM 457 C ALA 58 ATOM 458 O ALA 58 ATOM 459 N LYS 59 ATOM 460 CA LYS 59	21.884 41.136 -6.118 1.00 0.21 19.608 40.631 -6.871 1.00 0.21 19.393 41.275 -7.897 1.00 0.21 18.660 40.414 -5.941 1.00 0.31 17.329 40.910 -6.123 1.00 0.31	1SG 457 1SG 458 1SG 459 1SG 460 1SG 461
40	ATOM 462 CG LYS 59 ATOM 463 CD LYS 59 ATOM 464 CE LYS 59 ATOM 465 NZ LYS 59	16.237 39.929 -5.664 1.00 0.31 16.172 38.657 -6.511 1.00 0.31 15.844 38.913 -7.985 1.00 0.31 15.812 37.638 -8.834 1.00 0.31 15.485 37.972 -10.239 1.00 0.31	1SG 462 1SG 463 1SG 464 1SG 465 1SG 466
45	ATOM 467 O LYS 59 ATOM 468 N PHE 60 ATOM 469 CA PHE 60 ATOM 470 CB PHE 60	17.157 42.162 -5.331 1.00 0.31 18.068 42.622 -4.645 1.00 0.31 15.948 42.746 -5.431 1.00 0.23 15.595 43.928 -4.704 1.00 0.23 14.165 44.410 -4.999 1.00 0.23	1SG 467 1SG 468 1SG 469 1SG 470 1SG 471
50	ATCM 472 CD1 PHE 60 ATCM 473 CD2 PHE 60 ATCM 474 CE1 PHE 60 ATCM 475 CE2 PHE 60	13.854 45.482 -4.011 1.00 0.23 14.289 46.773 -4.202 1.00 0.23 13.119 45.189 -2.885 1.00 0.23 13.998 47.753 -3.282 1.00 0.23 12.825 46.165 -1.962 1.00 0.23	1SG 472 1SG 473 1SG 474 1SG 475 1SG 476
55	ATOM 477 C PHE 60 ATOM 478 O PHE 60 ATOM 479 N GLU 61 ATOM 480 CA GLU 61	13.264 47.451 -2.161 1.00 0.23 15.656 43.581 -3.255 1.00 0.23 16.056 44.387 -2.417 1.00 0.23 15.265 42.337 -2.942 1.00 0.15 15.215 41.816 -1.609 1.00 0.15	1SG 477 1SG 478 1SG 479 1SG 480 1SG 481
60	ATOM 482 CG GLU 61 ATOM 483 CD GLU 61 ATOM 484 OE1 GLU 61 ATOM 485 OE2 GLU 61	14.699 40.370 -1.604 1.00 0.15 15.521 39.448 -2.507 1.00 0.15 14.713 38.185 -2.765 1.00 0.15 14.026 37.714 -1.820 1.00 0.15 14.761 37.681 -3.919 1.00 0.15	1SG 482 1SG 483 1SG 484 1SG 485 1SG 486
65	ATOM 487 O GLU 61 ATOM 488 N ASP 62 ATOM 489 CA ASP 62 ATOM 490 CB ASP 62	16.595 41.837 -1.028 1.00 0.15 16.769 42.050 0.170 1.00 0.15 17.618 41.636 -1.877 1.00 0.16 18.983 41.538 -1.440 1.00 0.16 19.962 41.211 -2.582 1.00 0.16	1SG 487 1SG 488 1SG 489 1SG 490 1SG 491
70	ATOM 491 CG ASP 62 ATOM 492 OD1 ASP 62 ATOM 493 OD2 ASP 62	19.751 39.749 -2.954 1.00 0.16 18.944 39.075 -2.259 1.00 0.16 20.401 39.282 2.027	1SG 492 1SG 493 1SG 494

	ATOM	494 (19.4	37 42.80	01 -0.7	73 1.0	0 0.16	1SG 495
	MOTA MOTA	495 (496 N			20.29 18.90	99 42.74	49 0.1	00 1.0	0 0.16	1SG 496
5	MOTA	497	A SEF	63	19.35					1SG 497 1SG 498
3	MOTA MOTA		B SER		18.57 17.21	_	39 -1.05	50 1.0	0 0.20	15G 499
	ATOM	500 c			19.19	2 45.10				1SG 500
	MOTA MOTA	501 C			18.20	1 44.58	6 1.43	0 1.0		1SG 501 1SG 502
10	ATOM		A GLY	64 64	20.20 20.16				0.22	1SG 503
	MOTA MOTA	504 C 505 O		64	21.57	0 45.70	1 3.58	5 1.00		1SG 504 1SG 505
	MOTA	506 N		64 65	22.47 21.79					1SG 506
15	MOTA MOTA	507 C		65	23.11	5 45.55	7 5.43	6 1.00		1SG 507 1SG 508
	ATOM	508 C		65 65	23.19 22.86				0.19	1SG 509
	ATOM	510 C	D GLU	65	23.12	3 48.20				1SG 510 1SG 511
	MOTA MOTA		E1 GLU E2 GLU	65 65	22.72 23.73		6 9.22	5 1.00	0.19	1SG 512
20	ATOM	513 C	GLU	65	23.64					1SG 513
	ATOM ATOM	514 O 515 N	GLU	65	22.90	2 43.249	5 5.92	5 1.00		1SG 514 1SG 515
	ATOM	516 C	TYR TYR	66 66	24.976 25.570					1SG 516
25	A.TOM A.TOM	517 CE		66	26.312	42.202			0.22 0.22	1SG 517 1SG 518
20	ATOM	518 CG 519 CD	TYR 1 TYR	66 66	25.308 24.943				0.22	1SG 519
	ATOM	520 CD	2 TYR	66	24.726				0.22 0.22	1SG 520 1SG 521
	ATOM ATOM	521 CE 522 CE	1 TYR 2 TYR	66 66	24.019		1.440	1.00	0.22	1SG 521
30	ATOM.	523 CZ	TYR	66	23.446	41.606			0.22 0.22	1SG 523 1SG 524
		524 OH 525 C	TYR TYR	66 66	22.497		0.236	1.00	0.22	1SG 524 1SG 525
	ATOM	526 O	TYR	66	26.580 27.258				0.22 0.22	1SG 526
35		527 n 528 ca	LYS	67	26.683	41.768	7.516		0.45	1SG 527 1SG 528
		529 CB	LYS LYS	67 67	27.618 26.953	41.753 42.023			0.45	1SG 529
		530 CG	LYS	67	26.340	43.420	10.055	1.00 1.00	0.45 0.45	1SG 530 1SG 531
	-	531 CD 532 CE	LYS LYS	67 67	25.324 23.974	43.562 42.913	11.188	1.00	0.45	1SG 532
40		33 NZ	LYS	67	23.325	43.628	10.871 9.750	1.00 1.00	0.45 0.45	1SG 533 1SG 534
		534 C 535 O	LYS LYS	67 67	28.183 27.569	40.371 39.421	8.662	1.00	0.45	1SG 535
		36 N	CYS	68	29.390	40.228	8.180 9.244	1.00 1.00	0.45 0.52	1SG 536 1SG 537
45		37 CA 38 CB	CYS CYS	68 68	30.003 31.059	38.935	9.333	1.00	0.52	1SG 538
	ATOM 5	39 SG	CYS	68	32.113	38.703 37.291	8.250 8.666	1.00 1.00	0.52 0.52	1SG 539 1SG 540
		40 C 41 O	CYS CYS	68 68	30.754	38.840	10.621	1.00	0.52	1SG 541
	ATOM 5	42 N		69	31.295 30.796	39.830 37.631	11.110 11.218	1.00 1.00	0.52 0.27	1SG 542
50		43 CA 44 CB		69	31.610	37.462	12.382	1.00	0.27	1SG 543 1SG 544
		44 CB 45 CG		69 69	30.855 29.833	37.549 36.434	13.718 13.927	1.00	0.27	1SG 545
	ATOM 5	46 CD	GLN	69	29.290	36.575	15.342	1.00 1.00	0.27 0.27	1SG 546 1SG 547
55				69 69	29.847 28.177	37.306	16.160	1.00	0.27	1SG 548
	ATOM 5	49 C	GLN (59	32.221	35.853 36.103	15.642 12.322	1.00 1.00	0.27 0.27	1SG 549 1SG 550
		50 O		59 70	31.741 33.333	35.214	11.620	1.00	0.27	1SG 551
CO	ATOM 55	52 CA		0	33.988	35.928 34.660	13.056 13.145		0.11 0.11	1SG 552
60	ATOM 55 ATOM 55			0	35.166	33.594	10.252		0.11	1SG 553 1SG 554
	ATOM 55			0	35.399 35.405	34.688 34.631	11.056 12.551		0.11	1SG 555
	ATOM 55	6 NE2	HIS 7	0	35.486	35.325	8.894		0.11 0.11	1SG 556 1SG 557
65	ATOM 55 ATOM 55			0 0	35.593 35.229	35.736	10.211	1.00	0.11	1SG 558
	ATOM 55	9 C	HIS 7	0	34.110	34.031 34.372	8.970 14.599		0.11 0.11	1SG 559 1SG 560
	ATOM 56 ATOM 56	_	HIS 7 GLN 7	_	33.793 34.541	35.212	15.438	1.00	0.11	1SG 561
70	ATOM 56	2 CA	GLN 7	1	34.541 34.685	33.146 32.822	14.938 16.322		0.12 0.12	1SG 562
70	ATOM 56		GLN 7	1	35.169	31.379	16.553	1.00 0	0.12	1SG 563 1SG 564
		- 03	GLN 7		34.160	30.298	16.156	1.00	1.12	1SG 565

	ATOM	1 565	CD G	LN 71	33.10	0 30.21	2 17 24	10 1 0		
	ATOM	566	OE1 G	LN 71	33.03					1SG 566 1SG 567
	ATOM ATOM		NE2 G	LN 71 LN 71	32.23		6 17.17	1 1.0	0 0.12	1SG 568
5	ATOM	569	O G1		35.73 35.58					1SG 569
	ATOM ATOM		N GI		36.82	7 33.91	3 16.12			1SG 570 1SG 571
	ATOM		CA GI		37.95 39.12				0 0.21	1SG 572
10	ATOM		CG GI	N 72	39.53					1SG 573 1SG 574
10	ATOM ATOM		CD GI OE1 GI		39.80		16.49	8 1.0		1SG 574
	ATOM		NE2 GI		40.00 39.80					1SG 576
	ATOM		C GI		37.61	2 36.126	16.72			1SG 577 1SG 578
15	ATOM ATOM	578 579	O GL N VA		37.92 36.94				0.21	1SG 579
	ATOM	580	CA VA	L 73	36.75					1SG 580 1SG 581
	MOTA MOTA	581 582	CB VA		36.89		14.34	9 1.00		1SG 581
0.0	ATOM	583	CG2 VA		38.329 35.809					1SG 583
20	ATOM		C VA		35.419	38.532	16.245			1SG 584 1SG 585
	ATOM ATOM		O VAI N ASI		34.556 35.258			1.00	0.31	1SG 586
	ATOM	587	CA AS	N 74	34.078					1SG 587
25	ATOM ATOM		CB ASI CG ASI		34.389	41.966	17.323	1.00		1SG 588 1SG 589
	ATOM		CG ASI OD1 ASI		33.215 32.226		18.119 18.353		0.41	1SG 590
	ATOM		ND2 AS1	N 74	33.322	43.804	18.540		0.41 0.41	1SG 591 1SG 592
	ATOM ATOM		C Asi O Asi		33.177		15.647	1.00	0.41	1SG 593
30	ATOM	594 1	N GLU		33.389 32.113	39.959 41.457	14.644 15.746		0.41	1SG 594
	ATOM ATOM		CA GLU		31.220	41.642	14.641		0.48 0.48	1SG 595 1SG 596
	ATOM		CB GLU CG GLU		29.879 29.072	42.271 41.393	15.056		0.48	1SG 597
35	ATOM	598	D GLU	75	28.504	40.229	16.014 15.218	1.00	0.48 0.48	1SG 598 1SG 599
33	ATOM ATOM		DE1 GLU DE2 GLU		28.423	40.354	13.967	1.00	0.48	1SG 599
	ATOM	601			28.141 31.884	39.200 42.588	15.848 13.693	1.00 1.00	0.48	1SG 601
	ATOM ATOM	602 C			32.611	43.491	14.107	1.00	0.48 0.48	1SG 602 1SG 603
40	ATOM		I SER A SER		31.657 32.239	42.386 43.230	12.381	1.00	0.42	1SG 604
	ATOM		B SER	76	32.350	42.539	11.379 10.010	1.00	0.42 0.42	1SG 605 1SG 606
	ATOM ATOM	606 o	G SER	76 76	32.918 31.346	43.427	9.061	1.00	0.42	1SG 607
ΛE	ATOM	608 O	SER	76	30.182	44.416 44.388	11.208 11.604	1.00 1.00	0.42 0.42	1SG 608
45	ATOM ATOM	609 N 610 C		77	31.884	45.509	10.627	1.00	0.31	1SG 609 1SG 610
	ATOM	611 C		77 77	31.059 31.813	46.657 47.908	10.396 9.915	1.00	0.31	1SG 611
		612 C		77	32.856	48.431	10.898	1.00 1.00	0.31 0.31	1SG 612 1SG 613
50		613 C	D GLU E1 GLU	77 77	34.144 34.416	47.681	10.608	1.00	0.31	1SG 614
	ATOM	615 O	E2 GLU	77	34.871	47.430 47.348	9.403 11.581	1.00 1.00	0.31 0.31	1SG 615
		616 C 617 O	GLU GLU	77 77	30.149	46.280	9.278	1.00	0.31	1SG 616 1SG 617
		618 N	PRO	77 78	30. 4 93 28.978	45.470 46.839	8.419 9.296	1.00	0.31	1SG 618
55		619 CZ		78	28.046	46.505	8.257	1.00 1.00	0.29 0.29	1SG 619 1SG 620
		620 CI 621 CE		78 78	28.309 26.663	47.037	10.573	1.00	0.29	1SG 621
	ATOM (622 CG		78	26.830	46.846 46.701	8.806 10.328	1.00	0.29 0.29	1SG 622
60		523 C 524 O	PRO	78	28.349	47.178	6.959		0.29	1SG 623 1SG 624
		524 O 525 N	PRO VAL	78 79	28.956 27.945	48.248 46.539	6.958 5.845		0.29	1SG 625
		26 CA	VAL	79	28.075	47.100	4.536		0.31 0.31	1SG 626 1SG 627
	-	27 CB	VAL 1 VAL	79 79	28.861	46.242	3.590	1.00	0.31	15G 628
65	ATOM 6	29 CG	2 VAL	79 79	28.171 28.983	44.872 46.983	3.480 2.247		0.31	1SG 629
		30 C	VAL	79 70	26.678	47.181	4.020		0.31 0.31	1SG 630 1SG 631
		31 O 32 N	VAL TYR	79 80		46.245 48.306	4.193	1.00	0.31	1SG 632
70	ATOM 6	33 CA	TYR	80	24.946	48.385		1.00	0.19 0.19	1SG 633 1SG 634
70		34 CB 35 CG	TYR TYR	80 80	24.256	49.729	3.235	1.00 (0.19	1SG 635
			* * *	-	22.813	49.553	2.905	1.00 (0.19	1SG 636

5	ATOM 637 CD2 TYR 8 ATOM 638 CE1 TYR 8 ATOM 639 CE2 TYR 8	22.346 49.756 1.626 1.00 0.19 21.926 49.172 3.886 1.00 0.19 21.013 49.586 1.333 1.00 0.19 0 20.593 49.000 3.600 1.00 0.19	1SG 637 1SG 638 1SG 639
	3 0004 644	0 20.135 49.209 2.322 1.00 0.19 0 18.767 49.033 2.023 1.00 0.19 0 24.940 48.188 1.459 1.00 0.19 0 25.745 48.771 0.734 1.00 0.19	1SG 640 1SG 641 1SG 642 1SG 643 1SG 644
10	ATOM 645 CA LEU 8 ATOM 646 CB LEU 8 ATOM 647 CG LEU 8 ATOM 648 CD2 LEU 8	1 23.950 47.054 -0.424 1.00 0.08 1 24.024 45.551 -0.740 1.00 0.08 1 23.950 45.230 -2.243 1.00 0.08 1 23.763 43.724 -2.484 1.00 0.08	1SG 645 1SG 646 1SG 647 1SG 648 1SG 649
15	ATOM 650 C LEU 81 ATOM 651 O LEU 81 ATOM 652 N GLU 82 ATOM 653 CA GLU 82	1 25.157 45.810 -2.996 1.00 0.08 1 22.632 47.548 -0.923 1.00 0.08 1 21.611 47.411 -0.251 1.00 0.08 2 22.633 48.166 -2.119 1.00 0.09 2 21.417 48.652 -2.696 1.00 0.09	1SG 650 1SG 651 1SG 652 1SG 653
20	ATOM 654 CB GLU 82 ATOM 655 CG GLU 82 ATOM 656 CD GLU 82 ATOM 657 OE1 GLU 82 ATOM 658 OE2 GLU 82	21.424 50.176 -2.909 1.00 0.09 21.484 50.982 -1.610 1.00 0.09 21.724 52.442 -1.972 1.00 0.09 21.178 52.895 -3.014 1.00 0.09 22.467 53 122 -1.216 1.00 0.09	1SG 654 1SG 655 1SG 656 1SG 657 1SG 658
25	ATOM 659 C GLU 82 ATOM 660 O GLU 82 ATOM 661 N VAL 83 ATOM 662 CA VAL 83 ATOM 663 CB VAL 83	21.317 48.028 -4.048 1.00 0.09 1 22.273 48.049 -4.822 1.00 0.09 1 20.151 47.442 -4.369 1.00 0.09 1 19.999 46.839 -5.659 1.00 0.09 1 19.493 45.431 5 603 1.00 0.09 1	1SG 659 1SG 660 1SG 661 1SG 662 LSG 663
30	ATOM 664 CG1 VAL 83 ATOM 665 CG2 VAL 83 ATOM 666 C VAL 83 ATOM 667 O VAL 83 ATOM 668 N PHE 84	20.533 44.566 -4.871 1.00 0.09 1 18.111 45.445 -4.931 1.00 0.09 1 18.974 47.642 -6.383 1.00 0.09 1 17.973 48.052 -5.797 1.00 0.09 1	SG 664 SG 665 SG 666 SG 667 SG 668
35	ATOM 669 CA PHE 84 ATOM 670 CB PHE 84 ATOM 671 CG PHE 84 ATOM 672 CD1 PHE 84 ATOM 673 CD2 PHE 84	18.257 48.698 -8.403 1.00 0.23 1.08 1.09 1.00 0.23 1.09 1.00 0.23 1.09 1.00 1.00 1.00 1.00 1.00 1.00 1.00	SG 669 SG 670 SG 671 SG 672 SG 673
40	ATOM 674 CE1 PHE 84 ATOM 675 CE2 PHE 84 ATOM 676 CZ PHE 84 ATOM 677 C PHE 84 ATOM 678 O PHE 84	19.328 52.069 -5.740 1.00 0.23 18 21.428 51.294 -6.510 1.00 0.23 18 20.689 51.999 -5.594 1.00 0.23 18 17.966 47.967 -9.668 1.00 0.23 18	SG 674 SG 675 SG 676 SG 677 SG 678
45	ATOM 679 N SER 85 ATOM 680 CA SER 85 ATOM 681 CB SER 85 ATOM 682 OG SER 85 ATOM 683 C SER 85	16.802 48.247 -10.283 1.00 0.34 1s 16.544 47.653 -11.558 1.00 0.34 1s 15.248 46.824 -11.611 1.00 0.34 1s 14.121 47.637 -11.326 1.00 0.34 1s	G 679 G 680 G 681 G 682 G 683
50	ATOM 684 O SER 85 ATOM 685 N ASP 86 ATOM 686 CA ASP 86 ATOM 687 CB ASP 86 ATOM 688 CG ASP 86	15.403 49.431 -12.656 1.00 0.34 1s. 17.538 49.042 -13.267 1.00 0.23 1s. 17.542 50.101 -14.232 1.00 0.23 1s. 18.144 51.413 -13.702 1.00 0.23 1s.	G 684 G 685 G 686 G 687 G 688
55	ATOM 689 OD1 ASP 86 ATOM 690 OD2 ASP 86 ATOM 691 C ASP 86 ATOM 692 O ASP 86 ATOM 693 N TRP 87	15.949 51.949 -12.931 1.00 0.23 150 17.667 52.492 -11.625 1.00 0.23 150 18.413 49.652 -15.356 1.00 0.23 150 19.189 48.709 -15.213 1.00 0.23	G 689 G 690 G 691 G 692 G 693
60	ATOM 694 CA TRP 87 ATOM 695 CB TRP 87 ATOM 696 CG TRP 87 ATOM 697 CD2 TRP 87 ATOM 698 CD1 TRP 87	19.116 49.918 -17.626 1.00 0.14 1sg 18.696 50.502 -18.982 1.00 0.14 1sg 17.552 49.733 -19.589 1.00 0.14 1sg 17.711 48.410 -20.124 1.00 0.14 1sg	694 695 696 697 698
65	ATOM 699 NE1 TRP 87 ATOM 700 CE2 TRP 87 ATOM 701 CE3 TRP 87 ATOM 702 CZ2 TRP 87 ATOM 703 CZ3 TRP 87	15.562 49.008 -20.322 1.00 0.14 1sg 16.460 47.990 -20.570 1.00 0.14 1sg 18.813 47.610 -20.230 1.00 0.14 1sg 16.289 46.756 -21.133 1.00 0.14	699 700 701 702 703
70	ATOM 704 CH2 TRP 87 ATOM 705 C TRP 87 ATOM 706 O TRP 87	18.640 46.369 -20.801 1.00 0.14 1SG 17.402 45.949 -21.244 1.00 0.14 1SG 20.535 50.295 -17.364 1.00 0.14 1SG 21.443 49.504 -17.607 1.00 0.14 1SG	704 705 706

	ATOM	707 I	l LEU	88 20.	772 51.51	14 -16.84	7 1 00	0 10	
	ATOM		A LEU	88 22.	128 51.93	38 -16.64	9 1.00	0.12 0.12	1SG 708 1SG 709
	ATOM ATOM		B LEU G LEU		571 52.99	93 -17.67	9 1.00	0.12	1SG 710
5	ATOM		D2 LEU		277 54.75	34 -17.52 59 -18.34		0.12	1SG 711
	MOTA		D1 LEU	88 25.	038 52.37	77 -17.83	3 1.00 0 1.00	0.12 0.12	1SG 712
	ATOM ATOM	713 C		88 22.	224 52.58	4 -15.30	7 1.00	0.12	1SG 713 1SG 714
	ATOM	714 O		88 21. 89 23.		8 -14.85	6 1.00	0.12	1SG 715
10	ATOM	716 C		89 23.		2 -14.622 8 -13.352	2 1.00	0.11	1SG 716
	ATOM	717 C	_	89 23.	298 52.13	9 -12.138	2 1.00 3 1.00	0.11 0.11	1SG 717 1SG 718
	ATOM ATOM	718 C		89 23.	481 52.83	1 -10.774	1.00	0.11	1SG 718
	ATOM			89 23.1 89 22.				0.11	1SG 720
15	ATOM	721 C		89 24.		4 -10.560 4 -13.265	1.00	0.11	15G 721
	ATOM	722 0		89 25.1	347 52.94	9 -13.882	1.00	0.11 0.11	1SG 722 1SG 723
	MOTA MOTA	723 N 724 C		90 25.3	82 54.61	1 -12.507	1.00	0.11	15G 723
	ATOM	725 CI		90 26.5 90 26.6	28 55.04	6 -12.310		0.11	1SG 725
20	MOTA	726 C		90 28.1	46 57.033	6 -12.242 3 -12.047		0.11	1SG 726
	MOTA			90 28.2	28 58.537	7 -11.741		0.11 0.11	1SG 727 1SG 728
	ATOM ATOM	728 CI 729 C		90 29.0	13 56.629	-13.250		0.11	15G 728
	ATOM	730 o		90 26.8 90 26.1	75 54.478 67 54.707	-10.975		0.11	1SG 730
25	ATOM	731 N		27.9		7 -9.996 1 -10.903		0.11	1sg 731
	MOTA	732 CA		28.2	55 53.028			0.11 0.11	1SG 732 1SG 733
		733 CB 734 CG	-	01 28.6 01 27.4		-9.880		0.11	15G 734
20		735 CD		1 27.4 1 27.9	80 49 205	-10.484 -10.669		0.11	1SG 735
30			1 GLN 9	1 29.1	36 49.064	-11.026		0.11 0.11	1SG 736 1SG 737
		737 NE 738 C		1 27.0	99 48.288	-10.419		0.11	1SG 737
		739 0	GLN 9 GLN 9			-9.004	1.00	11	1SG 739
2 5		740 N	ALA 9			-9.654 -7.658).11	1SG 740
35		741 CA	ALA 9	2 30.44	6 54.291	-6.909).18).18	1SG 741 1SG 742
		742 CB 743 C	ALA 9: ALA 9:			-6.346	1.00 0	.18	1SG 743
		744 0	ALA 9			-5.743		- 18	1SG 744
40		745 N	SER 9	31.97		-5.231 -5.319		.18	1SG 745 1SG 746
40		746 CA 747 CB	SER 93			-4.192		.25	15G 747
		48 OG	SER 93			-3.991		.25	1SG 748
		49 C	SER 93		9 53.125	-2.865 -2.961		.25 .25	1SG 749
45		50 0	SER 93	31.11	3 52.443	-2.144		.25	1SG 750 1SG 751
10		51 N 52 CA	ALA 94 ALA 94			-2.798		.19	1SG 752
		53 CB	ALA 94		3 55.085 9 55.303	-1.611		. 19	1SG 753
		54 C	ALA 94			-0.534 -1.971		.19 .19	1SG 754
50		55 O 56 N	ALA 94		5 57.069	-2.923		. 19	1SG 755 1SG 756
		56 N 57 CA	GLU 95 GLU 95	29.81 29.16		-1.216	1.00 0.	. 12	1SG 757
	ATOM 7	58 CB	GLU 95	27.88		-1.400 -0.553		.12	1SG 758
		59 CG	GLU 95	26.823		-0.963		12	1SG 759 1SG 760
55		60 CD 61 OE1	GLU 95	25.743		0.108		12	1SG 761
		52 OE2		25.714 24.930				12	1SG 762
		53 C	GLU 95	30.096				12	1SG 763
	ATOM 76		GLU 95	30.230	60.228		1.00 0.	12 12	1SG 764 1SG 765
60	ATOM 76		VAL 96 VAL 96	30.780	59.047	0.164	1.00 0.	11	1SG 766
	ATOM 76		VAL 96	31.626 31.355	60.097 60.462		1.00 0.		1SG 767
	ATOM 76		VAL 96	32.367			1.00 0. 1.00 0.		1SG 768
	ATOM 76 ATOM 77	_		29.886	60.903	2.191	1.00 0.		1SG 769 1SG 770
65	ATOM 77		VAL 96 VAL 96	33.039 33.336	59.638	0.573	1.00 0.	11	1sg 771
	ATOM 77	_	VAL 97	33.336	58.455 60.587		1.00 0.1 1.00 0.1		1SG 772
	ATOM 77	3 CA '	VAL 97	35.339	60.254		1.00 0.1 1.00 0.1		1SG 773 1SG 774
	ATOM 77		VAL 97 VAL 97	35.826		-1.243 1	.00 0.1	10	1SG 775
70	ATOM 77	_		35.078 35.642		-2.062 1	.00 0.1	10	1SG 776
	ATOM 77		VAL 97	36.119	61.271		.00 0.1		1SG 777
							0.1	. •	1SG 778

	ATO	M 779	N M	AL 97 ET 98	35.60 37.40				1.10 1SG 779
_	ATO! ATO!			ET 98 ET 98	38.26 39.29		1.879	1.00 0	.12 1SG 781
5	ATON ATON		CG M	ET 98	38.65	60.261	3.835		.12 1SG 782 .12 1SG 783
	ATON			ET 98 ET 98	37.73 39.18		5.127	1.00 0	.12 15G 784
	ATOM		C M	ST 98	39.00				.12 1SG 785 .12 1SG 786
10	ATOM ATOM		O MI		39.18	8 62.048	-0.290	1.00 0	.12 1SG 787
	ATOM	788	CA GI		39.44 40.13		1.057 0.002		.10 1SG 788
	ATOM ATOM		CB GI		40.44	9 65.986	0.286		.10 1SG 789 .10 1SG 790
15	ATOM	791	CD GI	U 99	41.11 41.40		-0.906 -0.533		.10 1SG 791
13	ATOM ATOM		OE1 GI OE2 GI		40.50	0 68.797	0.034		.10 1SG 792 .10 1SG 793
	ATOM	794	C GI		42.54 41.42		-0.812 -0.211	1.00 0.	10 15G 794
	ATOM ATOM		O GL N GL		42.05	6 63.330	0.733		10 1sg 795 10 1sg 796
20	ATOM		CA GL		41.846 43.09		-1.486	1.00 0.	20 15G 797
	ATOM ATOM		C GL	Y 100	42.858	61.680	-1.803 -2.198		20 1SG 798 20 1SG 799
	ATOM		O GL		43.718		-2.822	1.00 0.	20 1SG 800
25	ATOM		CA GL	N 101	41.519		-1.860 -2.261	1.00 0. 1.00 0.	
20	ATOM ATOM		CB GLI CG GLI		40.589 39.119		-1.379	1.00 0.	
	ATOM	804	CD GL	V 101	38.416		-1.332 -0.499	1.00 0.1 1.00 0.1	50 1SG 804
	ATOM ATOM		DE1 GLI VE2 GLI		37.204	58.040	-0.574	1.00 0.9	
30	ATOM	807 (GL		39.213 41.046		0.318 -3.672	1.00 0.5	50 1SG 807
	MOTA MOTA	808 C			40.446	60.674	-4.176	1.00 0.5	
	ATOM	810 C	A PRO		41.375 40.964	58.654 58.525	-4.332 -5.698	1.00 0.5	7 1SG 810
35	ATOM ATOM	-	D PRO		42.668	58.028	-4.098	1.00 0.5 1.00 0.5	
	ATOM		B PRO G PRO		41.873 43.156	57.469 57.556	-6.321 -5.478	1.00 0.5	7 1SG 813
	MOTA ATOM	814 C 815 O			39.518	58.180	-5.764	1.00 0.5 1.00 0.5	
4.0	ATOM	816 N		102 103	39.021 38.823		-4.864	1.00 0.5	7 1SG 816
40	ATOM ATOM	817 C.		103	37.446	58.299	-6.818 -6.967	1.00 0.2 1.00 0.2	
	ATOM	818 C		103 103	36.529 35.043		-7.225	1.00 0.2	6 1SG 819
	ATOM ATOM		D2 LEU	103	34.221	** *		1.00 0.2 1.00 0.2	
45	ATOM	822 C	01 LEU LEU	103 103	34.473 37.366	58.542 57.422	-6.082	1.00 0.2	6 1SG 822
		823 o	LEU	103	37.940	·		1.00 0.20 1.00 0.20	
		824 N 825 C	PHE	104 104	36.674 36.542		-8.032	1.00 0.08	15G 825
50		826 CE	PHE	104	37.073			1.00 0.08 1.00 0.08	
30		827 CG 828 CD	PHE 1 PHE	104 104	37.001 37.981	53.256 -1	10.222	1.00 0.08	
	ATOM	829 CD	2 PHE	104	35.961	53.414 -1 52.393 -1		1.00 0.08 1.00 0.08	
		830 CE 831 CE	1 PHE 2 PHE	104 104	37.919 35.892	52.727 -1	12.365 1	1.00 0.08	
55	ATOM (832 CZ		104	36.873	51.703 -1 51.871 -1	11.664 1 12.611 1	1.00 0.08 1.00 0.08	
		833 C 934 O	PHE PHE	104	35.081	55.331 ~	9.441 1	1.00 0.08 1.00 0.08	
	ATOM 8	335 N	LEU	104 105	34.282 34.691	55.127 - 55.515 -1	8.528 1	.00 0.08	1SG 835
60	-	336 CA 37 CB	LEU	105	33.306	55.440 - 1	1.062 1	.00 0.10	1SG 836 1SG 837
		38 CG	LEU LEU	105 105	32.705 32.678	56.779 -1 57.865 -1	_	.00 0.10	1SG 838
			LEU	105	32.015	57.352 -	9.144 1	.00 0.10 .00 0.10	1SG 839 1SG 840
		40 CD1	LEU LEU	105 105	32.045 33.203	59.163 -10	0.958 1	.00 0.10	15G 841
65	ATOM 8	42 0	LEU	105	34.173	54.497 -12 54.269 -12	2.929 1	.00 0.10 .00 0.10	1SG 842 1SG 843
		43 N 44 CA	ARG ARG	106 106	32.014	53.900 -12	2.389 1.	.00 0.15	15G 844
	ATOM 8	45 CB	ARG	106		52.960 -13 51.519 -12	3.452 1. 2.938 1	.00 0.15 .00 0.15	1SG 845
70		46 CG 47 CD			31.891	50.409 -13	3.977 1.	00 0.15	1SG 846 1SG 847
		48 NE			32.273 <i>4</i> 32.035 <i>4</i>	49.049 -13 48.004 -14	3.387 1. 1.420 1	00 0.15	1SG 848
							*•	0.13	1SG 849

	ATO					31.10	8 47.03	2 -14.18	7 1.0	0 0.15	100 050
	ATO			1 AR			9 47.03	1 -13.00	9 1.0		1SG 850 1SG 851
	ATO ATO			2 AR				7 -15.11	9 1.0		1SG 852
5	ATO			AR		30.49 29.53		6 -14.00 7 -13.26			1SG 853
	ATO			CY	-	30.36		7 -13.26 8 -15.34	5 1.0 2 1.0		1SG 854 1SG 855
	ATO					29.05	9 53.09	6 -15.92	4 1.0		1SG 856
	ATO ATO					29.005		8 -17.25	5 1.0		1SG 857
10	ATO			CYS		29.607 28.730		2 -17.06			1SG 858
	ATO			CYS		29.442		8 -16.19 8 -16.92	0 1.00 7 1.00	_	1SG 859
	ATO			HIS	108	27.648	51.16	4 -15.57	2 1.00		1SG 860 1SG 861
	ATO			HIS		27.365	49.768	-15.70			1SG 862
15	ATO:			l HIS HIS		25.867		1 -14.34	3 1.00	0.11	1SG 863
	ATON			HIS		27.113 27.349	47.57	l -14.41° l -14.34°			1SG 864
	ATO	4 865		HIS		27.329		-14.542			1SG 865
	ATON			HIS		27.995	46.542	-14.54	1.00		1SG 866 1SG 867
20	ATOM ATOM			HIS		26.055	45.649	-14.420	1.00		1SG 868
	ATOM		_	HIS HIS		26.033 25.078		-16.350			1SG 869
	ATOM			GLY		25.949	48.636	-16.033 -17.287	1.00 1.00		1SG 870
	ATOM	_	CA	GLY		24.722		-17.976	1.00		1SG 871 1SG 872
25	ATOM		C	GLY		24.148	47.131	-17.403	1.00		1SG 872
20	ATOM ATOM		o N	GLY TRP	109 110	24.870	46.270	-16.904		0.09	1SG 874
	ATOM		CA	TRP	110	22.812 22.150		-17.469 -16.919			1SG 875
	ATOM		CB	TRP	110	20.623	46.057	-16.844	1.00		1SG 876
30	ATOM		CG	TRP	110	19.843	44.901	-16.269	1.00	0.32	1SG 877 1SG 878
30	ATOM ATOM			TRP	110	18.944	44.087	-17.034	1.00	0.32	1SG 879
	ATOM			TRP	110 110	19.782 18.904	44.442	-14.985	1.00	0.32	1SG 880
	ATOM			TRP	110	18.377		-14.905 -16.158	1.00	0.32	1SG 881
35	ATOM			TRP	110	18.613		-18.358	1.00	0.32 0.32	1SG 882 1SG 883
33	ATOM			TRP	110	17.467	42.241	-16.595	1.00	0.32	15G 884
	MOTA MOTA	884 885		TRP TRP	110	17.696		-18.796	1.00	0.32	1SG 885
	ATOM	886	C	TRP	110 110	17.134 22.469		-17.932 -17.783	1.00	0.32	1SG 886
4.0	ATOM	887	0	TRP	110	22.612	44.803	-18.999	1.00	0.32 0.32	1SG 887
40	ATOM	888	N	ARG	111	22.622		-17.146	1.00	0.53	1SG 888 1SG 889
	ATOM ATOM	889 890	CA	ARG	111	22.948		-17.835	1.00	0.53	1SG 890
	ATOM	891	CB CG	ARG ARG	111 111	21.891 20.728		-18.846	1.00	0.53	1SG 891
4.5	ATOM	892		ARG	111	19.970		-18.202 -19.176	1.00	0.53	1SG 892
45	ATOM	893		ARG	111	19.081		-20.019	1.00	0.53 0.53	1SG 893 1SG 894
	ATOM	894		ARG	111	18.507	40.481	-21.145	1.00	0.53	1SG 895
	ATOM ATOM	895 896	NH1 NH2		111	18.813	39.213	-21.550	1.00	0.53	1SG 896
_	ATOM	897		ARG	111 111	17.649 24.232	41.243 42.460		1.00	0.53	1SG 897
50	ATOM	898		ARG	111	24.532	41.678		1.00 1.00	0.53 0.53	1SG 898
	ATOM	899		ASN	112	25.038	43.468		1.00	0.33	1SG 899 1SG 900
	ATOM ATOM	900 901		ASN	112	26.311	43.678		1.00	0.33	1SG 901
	ATOM	902		asn Asn	112 112	27.335 27.731	42.576	-18.504	1.00	0.33	1SG 902
55	ATOM	903	OD1		112	28.052	42.721 · 43.819 ·	-17.046 -16 594	1.00	0.33	1SG 903
	ATOM	904	ND2		112	27.702	41.592	-16.288	1.00	0.33 0.33	1SG 904 1SG 905
	ATOM	905		ASN	112	26.153	43.727 -	-20.315	1.00	0.33	1SG 906
	ATOM ATOM	906 907		asn Trp	112	26.933	43.116 -		1.00	0.33	1SG 907
60	ATOM			rrp	113 113	25.146 25.015	44.464 - 44.533 -	-20.817	1.00	0.13	1SG 908
	ATOM			rrp	113		45.100 -	.22.240	1.00 1.00	0.13	1SG 909
	ATOM			rp	113		44.191 -		1.00	0.13 0.13	1SG 910 1SG 911
	ATOM		CD2 1			22.228	42.976 -	23.165	1.00	0.13	15G 911 15G 912
65	ATOM ATOM		CD1 T				44.306 -		1.00	0.13	1SG 913
			NE1 1 CE2 1				43.244 -			0.13	1SG 914
			CE3 I			21.075 22.895	42.416 - 42.373 -	22.619		0.13	1SG 915
	ATOM	916 (CZ2 T	RP			42.373 - 41.241 -			0.13 0.13	1SG 916
70		917 (CZ3 T	RP :	113	22.379	41.191 -			0.13	1SG 917 1SG 918
70			CH2 T			21.238	40.635 -	24.142	_	0.13	1SG 919
	MOTA	919 (T	RP :	113	26.119	45.405 -	22.742		0.13	1SG 920

	ATC ATC			TR				36 -22.03		0.13	1SG 921
	ATO							27 -24.02 75 -24.57			1SG 922
5	ATC			B AS	P 114			33 -26.05	1 1.0 9 1.0		1SG 923 1SG 924
5	ATC ATC		_				4 44.24	11 -26.18	9 1.0	0 0.12	18G 925
	ATO		_	01 AS: 02 AS:				75 -25.53 16 -26.95	1 1.0		1SG 926
	ATO	M 92	7 C	AS		27.24		3 -24.47		_	15G 927
10	ATO			AS		26.13		8 -24.80	3 1.0		1SG 928 1SG 929
10	ATO ATO			LAV LA.V		28.21		2 -23.99	9 1.0	0 0.21	1SG 930
	ATO					27.97; 27.896		7 -23.88 1 -22.46			1SG 931
	ATO			1 VAI		27.643		9 -22.48	$\begin{array}{cccccccccccccccccccccccccccccccccccc$		1SG 932 1SG 933
15	OTA OTA			2 VAI		26.813	3 49.31	7 -21.72	8 1.0		1SG 933
10	ATO			VAI VAI		29.128 30.265		6 -24.51	6 1.00		1SG 935
	ATO	-		TYF		28.848		3 -24.44 3 -25.17			1SG 936
	ATO					29.880		4 -25.80	4 1.00		1SG 937 1SG 938
20	ATO ATO					30.062	51.87	4 -27.28	3 1.00		15G 939
20	ATON			TYR 1 TYR		28.712 28.279		7 -27.883	1.00		1SG 940
	ATON			2 TYR		27.864	50.200	0 -28.399 9 -27.902	1.00 1.00		1SG 941
	ATOM			1 TYR		27.023	53.311	1 -28.945	1.00		1SG 942 1SG 943
25	ATOM ATOM				116	26.607	51.031	1 -28.445	1.00		1SG 943
20	ATOM			TYR TYR	116 116	26.183 24.892	52.225	-28.971	1.00	0.44	1SG 945
	ATOM			TYR	116	29.464		2 -29.530 3 -25.712			1SG 946
	ATOM			TYR	116	28.359	53.962	25.263	1.00		1SG 947 1SG 948
30	ATOM ATOM			LYS	117	30.353	54.580	-26.142	1.00		1SG 949
	ATOM			LYS	117 117	30.080 29.019		-26.073			1SG 950
	ATOM		CG	LYS	117	29.519	56.616	-27.064 -28.501	1.00	0.45	1SG 951
	ATOM		CD	LYS	117	28.443	57.089	-29.479	1.00	0.45 0.45	1SG 952 1SG 953
35	ATOM ATOM		CE NZ	LYS	117	28.988	57.432	-30.865	1.00	0.45	1SG 954
	ATOM	_	C	LYS LYS	117 117	29.035 29.606		-31.705	1.00	0.45	1SG 955
	MOTA	956	0	LYS	117	28.453		-24.702 -24.513	1.00	0.45 0.45	1SG 956
	ATOM		N	VAL	118	30.497	56.195	-23.704	1.00	0.21	1SG 957 1SG 958
40	ATOM ATOM	958 959	CA CB	VAL VAL	118 118	30.122	56.475	-22.352	1.00	0.21	1SG 959
	ATOM	960		VAL	118	30.761 30.419		-21.370 -19.953	1.00	0.21	1SG 960
	MOTA	961	CG2	VAL	118	30.294	54.109	-21.678	1.00	0.21 0.21	1SG 961 1SG 962
	ATOM ATOM	962	C	VAL	118	30.579	57.856	-22.012	1.00	0.21	15G 963
45	MOTA	963 964	O N	VAL ILE	118 119	31.688		-22.354	1.00	0.21	1SG 964
	ATOM	965	CA	ILE	119	29.704 30.083		-21.340 -20.951	1.00	0.09	1SG 965
	ATOM	966	CB	ILE	119	29.298		-21.637	1.00	0.09 0.09	1SG 966 1SG 967
	ATOM	967		ILE	119	29.724	62.381	-21.035	1.00	0.09	1SG 968
50	MOTA MOTA	968 969	CG1 CD1		119 119	29.490		-23.159	1.00	0.09	1SG 969
	ATOM	970	C	ILE	119	28.509 29.821	60 088	-23.947 -19.488	1.00	0.09	1SG 970
	ATOM	971	0	ILE	119	28.827	59.579	-18.972	1.00 1.00	0.09 0.09	1SG 971 1SG 972
	MOTA MOTA	972	N	TYR	120	30.737	60.771	-18.778	1.00	0.09	1SG 973
55	ATOM	973 974	CA CB	TYR TYR	120 120	30.560 31.820	61.006	-17.378	1.00	0.09	1SG 974
	ATOM	975	CG	TYR	120	31.970	59.317	-16.525 -16.261	1.00 1.00	0.09	1SG 975
	MOTA	976		TYR	120	32.530	58.457	-17.178	1.00	0.09 0.09	1SG 976 1SG 977
	ATOM ATOM	977 978	CD2		120	31.540	58.817	-15.054	1.00	0.09	1SG 978
60	MOTA	979	CE1 CE2		120 120	32.652	57.117		1.00	0.09	1SG 979
	MOTA	980		TYR	120	31.659 32.217	57.483 - 56.631 -		1.00	0.09	1SG 980
	ATOM	981	OH	TYR	120		55.263	-15.355	1.00	0.09 0.09	1SG 981 1SG 982
	MOTA MOTA	982			120	30.176	62.434 -	-17.220	1.00	0.09	15G 983
65	ATOM	983 984			120 121	30.750 29.163	63.318 -	-17.855	1.00	0.09	1SG 984
	ATOM	985					62.691 - 64.038 -	-16.372 -16.102	1.00	0.18	1SG 985
	ATOM	986	CB :	L YR	121		64.245 -		1.00	0.18 0.18	1SG 986 1SG 987
	ATOM ATOM	987 988				27.150	63.949 -	18.056	1.00	0.18	1SG 988
70	ATOM		CD1 1 CD2 1				64.931 -			0.18	1SG 989
			CE1				62.683 - 64.654 -	. 10.486 . 20.337		0.18	1SG 990
								,	1.00	0.18	1SG 991

	ATOM 991 CE2 TYR 121 ATOM 992 CZ TYR 121 ATOM 993 OH TYR 121	26.942 63.389 -20.756 1.00 0.18	1SG 992 1SG 993
5	ATOM 994 C TYR 121 ATOM 995 O TYR 121 ATOM 996 N LYS 122 ATOM 997 CA LYS 122	28.829 64.371 -14.740 1.00 0.18 28.541 63.547 -13.874 1.00 0.18 29.284 65.605 -14.456 1.00 0.38	1SG 994 1SG 995 1SG 996 1SG 997
10	ATOM 998 CB LYS 122 ATOM 999 CG LYS 122 ATOM 1000 CD LYS 122	30.880 66.537 -12.818 1.00 0.28 31.137 66.957 -11.369 1.00 0.28 32.608 67.287	1SG 998 1SG 999 1SG1000
	ATOM 1001 CE LYS 122 ATOM 1002 NZ LYS 122 ATOM 1003 C LYS 122 ATOM 1004 O LYS 122	33.591 66.393 -11.855 1.00 0.28 34.985 66.786 -11.541 1.00 0.28 28.641 67.394 -13.143 1.00 0.28	1SG1001 1SG1002 1SG1003 1SG1004
15	ATOM 1005 N ASP 123 ATOM 1006 CA ASP 123 ATOM 1007 CB ASP 123	27.517 67.417 -12.408 1.00 0.20 26.698 68.590 -12.349 1.00 0.20 27.342 69.736 -11.555 1.00 0.20	1SG1005 1SG1006 1SG1007
20	ATOM 1008 CG ASP 123 ATOM 1009 OD1 ASP 123 ATOM 1010 OD2 ASP 123 ATOM 1011 C ASP 123	27.300 69.305 -10.096 1.00 0.20 26.407 68.486 -9.750 1.00 0.20 28.159 69.781 -9.310 1.00 0.20 26.373 69.035 3.70	1SG1008 1SG1009 1SG1010 1SG1011
25	ATOM 1012 O ASP 123 ATOM 1013 N GLY 124 ATOM 1014 CA GLY 124	26.275 70.230 -14.018 1.00 0.20 26.196 68.062 -14.652 1.00 0.17 25.784 68.369 -15.990 1.00 0.17	1SG1012 1SG1013 1SG1014 1SG1015
	ATOM 1016 0 GLY 124 ATOM 1017 N GLU 125 ATOM 1018 CA GLU 125	26.969 68.690 -16.840 1.00 0.17 26.818 69.053 -18.006 1.00 0.17 28.189 68.566 -16.293 1.00 0.24	1SG1013 1SG1016 1SG1017 1SG1018
30	ATOM 1019 CB GLU 125 ATOM 1020 CG GLU 125 ATOM 1021 CD GLU 125 ATOM 1022 OE1 GLU 125	30.365 69.739 -16.386 1.00 0.24 31.381 70.369 -17.331 1.00 0.24 32.334 71.210 -16.497 1 00 0.24	1SG1019 1SG1020 1SG1021 1SG1022
35	ATOM 1023 OE2 GLU 125 ATOM 1024 C GLU 125 ATOM 1025 O GLU 125	32.807 72.256 -17.015 1.00 0.24 29.961 67.582 -17.482 1.00 0.24 30.165 66.716 -16.637 1.00 0.24	1SG1023 1SG1024 1SG1025
40	ATOM 1027 CA ALA 126 ATOM 1028 CB ALA 126 ATOM 1029 C ALA 126	30.306 67.396 -18.766 1.00 0.26 30.860 66.125 -19.130 1.00 0.26 30.790 65.834 -20.639 1.00 0.26 32.302 66.112 13.742	18G1026 1SG1027 1SG1028 1SG1029
40	ATOM 1030 O ALA 126 ATOM 1031 N LEU 127 ATOM 1032 CA LEU 127 ATOM 1033 CB LEU 127	33.114 66.845 -19.302 1.00 0.26 32.645 65.289 -17.731 1.00 0.39 34.008 65.183 -17.302 1.00 0.39	15G1030 15G1031 15G1032 15G1033
45	ATOM 1034 CG LEU 127 ATOM 1035 CD2 LEU 127 ATOM 1036 CD1 LEU 127	33.482 64.807 -14.812 1.00 0.39 13.3881 63.986 -13.576 1.00 0.39 13.960 64.884 -15.010 1.00 0.39	lsG1034 lsG1035 lsG1036
50	ATOM 1038 O LEU 127 ATOM 1039 N LYS 128	34.796 64.549 -18.400 1.00 0.39 1 35.840 65.061 -18.800 1.00 0.39 1 34.304 63.411 -18.933 1.00 0.42	.SG1037 .SG1038 .SG1039 SG1040
	ATCM 1041 CB LYS 128 ATCM 1042 CG LYS 128 ATCM 1043 CD LYS 128	36.120 61.788 -19.443 1.00 0.43 1 35.512 60.519 -18.844 1.00 0.43 1 36.528 59.394 -18.642 1.00 0.43	SG1041 SG1042 SG1043 SG1044
55	ATOM 1045 NZ LYS 128 ATOM 1046 C LYS 128 ATOM 1047 O LYS 128	35.161 57.519 -19.451 1.00 0.43 1: 34.135 61.974 -20.820 1.00 0.43 1: 34.135 61.974 -20.820 1.00 0.43 1:	SG1045 SG1046 SG1047
60	ATOM 1048 N TYR 129 3 ATOM 1049 CA TYR 129 3 ATOM 1050 CB TYR 129 3	14.557 61.737 -22.075 1.00 0.26 15 13.811 60.931 -22.993 1.00 0.26 15 3.135 61.748 -24.108 1.00 0.26	5G1048 5G1049 5G1050 5G1051
65	ATOM 1052 CD1 TYR 129 3 ATOM 1053 CD2 TYR 129 3 ATOM 1054 CE1 TYR 129 3	2.73 60.810 -25.201 1.00 0.26 1s 1.645 59.997 -25.109 1.00 0.26 1s 3.524 60.758 -26.339 1.00 0.26 1s 1.320 59.142 -26.139 1.00 0.26 1s	G1052 G1053 G1054
	ATOM 1056 CZ TYR 129 33 ATOM 1057 OH TYR 129 33	3.205 59.908 -27.369 1.00 0.26 1s 2.101 59.099 -27.271 1.00 0.26 1s 1.779 58.229 -28.332 1.00 0.26 1s	G1055 G1056 G1057 G1058
70	ATOM 1059 0 TYR 129 35 ATOM 1060 N TRP 130 34	5.824 60.422 -24.135 1.00 0.26 1sc 1.462 58.689 -23.653 1.00 0.16 1sc	G1059 G1060 G1061
		-110 0.10 150	F1062

	ATOM	1062 0	B TRE	130	26 21	7 57 6				
	ATOM				36.31 37.41		50 -23.3° 04 -24.08	76 1.0		1SG1063
	ATOM		D2 TRP	130	38.74		20 -24.26	35 1.0 53 1.0		1SG1064
5	MOTA MOTA		D1 TRP		37.41	1 55.05	4 -24.63	30 1.0		1SG1065 1SG1066
J	ATOM		E1 TRP	130 130	38.65	1 54.76	5 -25.14	16 1.00		1SG1067
	ATOM			130	39.48 39.30		0 -24.92	3 1.00		1SG1068
	ATOM	1069 C		130	40.79		1 -23.90 5 -25.23	00 1.00 12 1.00		1SG1069
10	ATOM			130	40.63		6 -24.21			1SG1070 1SG1071
10	ATOM ATOM			130	41.36	4 57.23	7 -24.87	2 1.00		1SG1071
	ATOM	1072 C	TRP TRP	130 130	34.44 33.46	5 56.71	0 -24.89	_	0.16	1SG1073
	ATOM	1074 N	TYR	131	34.74		2 -24.27 1 -26.12	0 1.00		1SG1074
15	ATOM	1075 C		131	33.87	55.24	2 -26.12 2 -26.67	$ \begin{array}{cccc} 0 & 1.00 \\ 1 & 1.00 \end{array} $		18G1075
15	ATOM ATOM	1076 CI		131	34.25	54.83	0 -28.10	2 1.00		1SG1076 1SG1077
	ATOM	1077 CC 1078 CI	TYR	131 131	33.89		3 -29.04		0.17	1SG1078
	ATOM	1079 CI	2 TYR	131	34.67° 32.77°		1 -29.15 1 -29.83			1SG1079
20	ATOM	1080 CE	E1 TYR	131	34.335	58.049	9 -30.04	3 1.00 0 1.00	0.17 0.17	1SG1080
20	ATOM	1081 CE		131	32.430	56.794	4 -30.71	5 1.00	0.17	1SG1081 1SG1082
	MOTA MOTA	1082 CZ 1083 OH		131	33.211	57.920	-30.82	1 1.00	0.17	1SG1082
	ATOM	1084 C	TYR	131 131	32.855 33.952	58.940	-31.729		0.17	1SG1084
0.5	ATOM	1085 o	TYR	131	32.949	53.520	-25.858 -25.323	1.00	0.17	1sG1085
25	ATOM	1086 N	GLU	132	35.164	53.409	-25.753	1.00	0.17 0.19	1SG1086 1SG1087
	ATOM ATOM	1087 CA 1088 CB		132	35.336	52.145	-25.095	1.00	0.19	15G1087
	ATOM	1089 CG		132 132	36.595 37.918	51.383	-25.550	1.00	0.19	1SG1089
2.0	ATOM	1090 CD	GLU	132	39.023	51.244	-25.259 -25.885		0.19	1SG1090
30	ATOM	1091 OE	1 GLU	132	38.999	49.998	-25.702	1.00	0.19 0.19	1SG1091
	atom Atom	1092 OE:		132	39.905	51.838	-26.561	1.00	0.19	1SG1092 1SG1093
	ATOM	1094 0	GLU GLU	132 132	35.334 34.804	52.226	-23.595		0.19	1SG1094
2.5	ATOM	1095 N	ASN	133	35.901	53 300	-22.938 -23.008	1.00	0.19	1SG1095
35	MOTA	1096 CA	ASN	133	36.132	53.303	-21.586	1.00 1.00	0.18 0.18	1SG1096
	ATOM	1097 CB	ASN	133	37.146	54.366	-21.119	1.00	0.18	1SG1097 1SG1098
	ATOM ATOM	1098 CG 1099 OD1	ASN	133	37.569	54.017	-19.697	1.00	0.18	1SG1099
		1100 ND2	ASN ASN	133 133	36.964 38.631	53.162	-19.050 -19.191	1.00	0.18	1SG1100
40	ATOM	1101 C	ASN	133	34.876	53.504	-19.191	1.00 1.00	0.18	1SG1101
	ATOM	1102 0	ASN	133	34.256	54.566	-20.828	1.00	0.18 0.18	1SG1102 1SG1103
	MOTA MOTA	1103 N 1104 CA		134	34.477	52.431	-20.089	1.00	0.16	1SG1103
		1105 ND1	HIS	134 134	33.342 31.445		-19.214	1.00	0.16	1SG1105
45	MOTA	1106 CG		134	32.655	50.137	-20.751 -20.093	1.00 1.00	0.16	1SG1106
		1107 CB	HIS	134	32.970	50.911	-18.870	1.00	0.16 0.16	1SG1107 1SG1108
	ATOM ATOM	1108 NE2 1109 CD2	HIS	134	32.738	48.717	-21.871	1.00	0.16	15G1108
		1110 CE1		134 134	33.432 31.550	49.231	-20.790	1.00	0.16	1SG1110
50		1111 c		134	33.620	49.291 53.068	-21.805 -17 020	1.00	0.16	1SG1111
	ATOM	1112 0	HIS :	L34	32.711	53.632	-17.314	1.00 1.00	0.16 0.16	1SG1112
		1113 N 1114 CA		135	34.887	53.046	-17.453		0.14	1SG1113 1SG1114
		1114 CA			35.191	53.542	-16.136	1.00	0.14	1SG1115
55	ATOM 1	1116 CG			36.182 35.543	52.646 · 51.277 ·	-15.379		0.14	1SG1116
	ATOM 1	1117 OD1	ASN 1		34.446	51.144	-14.676		0.14 0.14	1SG1117
		118 ND2			36.246	50.224 -	-15.714		0.14	1SG1118 1SG1119
		119 C 120 O			35.824	54.896 -	-16.197	1.00	0.14	1SG1120
60		121 N			36.357 35.735	55.313 - 55.630 -	17.223		0.14	1SG1121
	ATOM 1	122 CA		4 .		56.921 -	13.065		0.19	1SG1122
		123 CB	ILE 1	36 :	35.366	58.059 -	14.963		0.19 0.19	1SG1123 1SG1124
	ATOM 1 ATOM 1	124 CG2 125 CG1			34.435	57.932 -	13.746	1.00 (.19	1SG1124 1SG1125
65	ATOM 1	125 CG1 126 CD1	17.E 1		36.110	59.402 -	15.040	1.00	.19	1SG1126
	ATOM 1				35.202 36.965	60.579 - 56.952 -	15.391		1.19	1SG1127
	ATOM 1	128 O	ILE 1		6.449	56.350 -			.19 .19	1SG1128
	ATOM 1:			37 3	8.112	57.642 -	13.419		.24	1SG1129 1SG1130
70					8.739	57.700 -	12.133	1.00 0	.24	1SG1131
					9.970 :	56.783 -: 56.873 -:			.24	1SG1132
				•			10.143	1.00 0	.24	1SG1133

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	ATOM 1133 C SER	137 39.198	59.104 -11.9	07 1 00 0 04	
	ATOM 1134 O SER	137 39.686	59.763 -12.8	23 1.00 0.24	1SG1134 1SG1135
	ATOM 1135 N ILE ATOM 1136 CA ILE	138 39.035 138 39.486	59.607 -10.6	70 1.00 0.31	1SG1136
5	ATOM 1137 CB ILE	138 38.419	60.933 -10.3 61.805 -9.7		1SG1137
	ATOM 1138 CG2 ILE	138 39.058	63.162 -9.4	43 1.00 0.31	1SG1138 1SG1139
	ATOM 1139 CG1 ILE ATOM 1140 CD1 ILE	138 37.227	61.911 -10.75	57 1.00 0.31	1SG1139
	ATOM 1141 C ILE	138 35.963 138 40.547	62.479 -10.11 60.785 -9.34		1SG1141
10	ATOM 1142 O ILE	138 40.328	60.785 -9.34 60.190 -8.29		1SG1142
	ATOM 1143 N THR ATOM 1144 CA THR	139 41.743	61.328 -9.61		1SG1143 1SG1144
	ATOM 1144 CA THR ATOM 1145 CB THR	139 42.788 139 44.128	61.172 -8.64	8 1.00 0.40	1SG1145
1 -	ATOM 1146 OG1 THR	139 44.128	60.908 -9.26 61.963 -10.14		1SG1146
15	ATOM 1147 CG2 THR	139 44.075	59.569 -10.01	9 1.00 0.40 3 1.00 0.40	15G1147 1SG1148
		139 42.873	62.438 -7.87		15G1148
	3.0004 - 4.4.4.	139 42.513 140 43.351	63.503 -8.36		1SG1150
20	ATOM 1151 CA ASN	140 43.471	62.333 -6.61 63.472 -5.75	3 1.00 0.29 0 1.00 0.29	1SG1151
20	3	140 44.596	64.437 -6.16		1SG1152 1SG1153
		140 45.928 140 46.306	63.762 -5.86	8 1.00 0.29	1SG1154
	ATOM 1155 ND2 ASN	140 46.306 140 46.667	62.785 -6.51 64.304 -4.86		1SG1155
25	ATOM 1156 C ASN	140 42.181	64.224 -5.75		1SG1156
23		40 42.115	65.358 -6.22	6 1.00 0.29	1SG1157 1SG1158
	3000 1450	41 41.113 41 39.821	63.595 -5.22	7 1.00 0.26	1SG1159
	ATOM 1160 CB ALA 1	41 38.719	64.215 -5.216 63.333 -4.603		1SG1160
30		41 39.898	65.471 -4.413		1SG1161 1SG1162
30		41 40.719 42 39.031	65.603 -3.507	1.00 0.26	1SG1163
	3	42 39.031 42 38.998	66.442 -4.762 67.708 -4.097		1SG1164
	ATOM 1165 CB THR 1	42 39.528	68.833 -4.935		1SG1165 1SG1166
35	3 mon / 4 4 4 m	42 39.621	70.022 -4.165	1.00 0.35	1SG1167
		42 38.582 42 37.569	69.043 -6.130 68.019 -3.789		1SG1168
	ATOM 1169 0 THR 1	42 36.665	68.019 -3.789 67.266 -4.145		1SG1169
			69.150 -3.095		1SG1170 1SG1171
40	3000		69.574 -2.700		1SG1172
	ATOM 1173 CG1 VAL 1	4	70.811 -1.856 71.189 -1.502	1.00 0.29 1.00 0.29	1SG1173
		36.953	70.542 -0.631	1.00 0.29	1SG1174 1SG1175
	ATOM 1175 C VAL 14 ATOM 1176 O VAL 14		69.861 -3.926	1.00 0.29	1SG1176
45	ATOM 1177 N GLU 14		69.598 -3.970 70.403 -4.967	1.00 0.29	1SG1177
	ATOM 1178 CA GLU 14		70.752 -6.183	1.00 0.25 1.00 0.25	1SG1178 1SG1179
	ATOM 1179 CB GLU 14 ATOM 1180 CG GLU 14		71.376 -7.228	1.00 0.25	15G1179 1SG1180
	ATOM 1180 CG GLU 14 ATOM 1181 CD GLU 14		72.746 -6.801	1.00 0.25	1SG1181
50	ATOM 1182 OE1 GLU 14		72.520 -5.676 72.013 -5.971	1.00 0.25 1.00 0.25	1SG1182
	ATOM 1183 OE2 GLU 14	4 37.326 7	2.845 -4.507	1.00 0.25	1SG1183 1SG1184
	ATOM 1184 C GLU 14 ATOM 1185 O GLU 14		9.501 -6.767	1.00 0.25	1SG1185
p	ATOM 1186 N ASP 14		9.521 -7.417 8.367 -6.525	1.00 0.25	1SG1186
55	ATOM 1187 CA ASP 14	5 34.927 6	7.107 -7.086	1.00 0.22 1.00 0.22	15G1187 1SG1188
	ATOM 1188 CB ASP 14. ATOM 1189 CG ASP 14.	5 35.835 6	5.959 -6.608	1.00 0.22	1SG1188
	ATOM 1189 CG ASP 148 ATOM 1190 OD1 ASP 148		4.709 -7.427	1.00 0.22	1SG1190
~ 0	ATOM 1191 OD2 ASP 145		4.287 -7.484 4.160 -8.016	1.00 0.22 1.00 0.22	1SG1191
60	ATOM 1192 C ASP 145	33.523 6	6.785 -6.680	1.00 0.22 1.00 0.22	1SG1192 1SG1193
	ATOM 1193 0 ASP 145 ATOM 1194 N SER 146		6.255 -7.486	1.00 0.22	1SG1194
	ATOM 1195 CA SER 146		7.103 -5.430 6.766 -4.974	1.00 0.20	1SG1195
65	ATOM 1196 CB SER 146		5.766 -4.974 7.291 -3.563	1.00 0.20 1.00 0.20	1SG1196
65	ATOM 1197 OG SER 146 ATOM 1198 C SER 146	31.476 68	3.711 -3.564	1.00 0.20	1SG1197 1SG1198
	ATOM 1198 C SER 146 ATOM 1199 O SER 146		7.344 -5.914	1.00 0.20	1SG1199
	ATOM 1200 N GLY 147		3.414 -6.488 5.614 -6.114	1.00 0.20	1SG1200
70	ATOM 1201 CA GLY 147	28.676 67	-077 -7.012	1.00 0.21 1.00 0.21	1SG1201 1SG1202
70	ATOM 1202 C GLY 147 ATOM 1203 O GLY 147	27.818 65	.904 -7.348	1.00 0.21	1SG1202 1SG1203
	ATOM 1203 O GLY 147	27.869 64	.869 -6.686	1.00 0.21	1SG1204

	ATOM 1204 N THR 148	
	ATOM 1204 N THR 148 ATOM 1205 CA THR 148	26.991 66.048 -8.399 1.00 0.17 1SG1205
	ATOM 1206 CB THR 148	20.137 64.966 -8.774 1.00 0.17 1SG1206
5	ATOM 1207 OG1 THR 148	24.174 66 037 7 033 1.00 0.17 1SG1207
5	ATOM 1208 CG2 THR 148	23 912 64 152 1.00 U.1/ 1SG1208
	ATOM 1209 C THR 148 ATOM 1210 O THR 148	26.701 64.381 -10.022 1.00 0.17 1561209
	ATOM 1210 O THR 148 ATOM 1211 N TYR 149	27.063 65.103 -10.949 1.00 0.17 1861210
	ATOM 1212 CA TYR 149	27 360 63.040 -10.068 1.00 0.12 1SG1212
10	ATOM 1213 CB TYR 149	28 585 61 526 12 231 1.00 0.12 1SG1213
	ATOM 1214 CG TYR 149	29.753 62.381 -10.600 1.00
	ATOM 1215 CD1 TYR 149 ATOM 1216 CD2 TYR 149	29.899 62.900 -9.335 1.00 0 12 1561213
	3.000 4.040	30.712 62.647 -11.548 1.00 0.12 1561217
15	ATOM 1217 CE1 TYR 149 ATOM 1218 CE2 TYR 149	30.988 63.680 -9.026 1.00 0.12 1501210
	ATOM 1219 CZ TYR 149	31 940 63 945 -11.245 1.00 0.12 1SG1219
	ATOM 1220 OH TYR 149	33.057 64.744 -9.663 1.00 0.12 1SG1220
	ATOM 1221 C TYR 149	26.341 61.495 -11 819 1 00 0.12 1SG1221
20	ATOM 1222 O TYR 149 ATOM 1223 N TYR 150	25.587 60.836 -11.105 1.00 0 12 1551222
	ATOM 1223 N TYR 150 ATOM 1224 CA TYR 150	26.286 61.458 -13.164 1.00 0.12 1551223
	ATOM 1225 CB TYR 150	25.436 60.528 -13.842 1.00 0 12 1561225
	ATOM 1226 CG TYR 150	21.020 61.036 -14.1/7 1.00 0.12 1561226
25	ATOM 1227 CD1 TYR 150	24.135 62.078 =16.450 1.00 0.12 1SG1227
23	ATOM 1228 CD2 TYR 150	24.090 63 507 14 550 4 55
	ATOM 1229 CE1 TYR 150 ATOM 1230 CE2 TYR 150	24.184 63.175 -17.277 1.00 0.12 1501229
	ATOM 1230 CE2 TYR 150 ATOM 1231 CZ TYR 150	24.140 64.607 -15.380 1.00 0 12 1861221
20	ATOM 1232 OH TYR 150	24 236 65 500 17 500 0.12 1SG1232
30	ATOM 1233 C TYR 150	26.154 60 142 15 000 1 7
	ATOM 1234 O TYR 150	27.127 60 786 -15 483 1.00 0.12 ISG1234
	ATOM 1235 N CYS 151 ATOM 1236 CA CYS 151	25.714 59.054 -15.747 1.00 0 27 1801236
	ATOM 1236 CA CYS 151 ATOM 1237 CB CYS 151	26.449 58.615 -16.891 1.00 0.27 1801237
35	ATOM 1220 OF SUB-151	27.202 57.301 -16.613 1.00 0.27 1991323
	ATOM 1239 C CYS 151	25.494 58 381 -18 012 1.00 0.27 1SG1239
	ATOM 1240 O CYS 151	24.314 58 113 17 70m 1.00 0.27 ISG1240
		25.991 58.533 -19.254 1.00 0.37 1001241
40	3.TOM 1242 CD	25.213 58.239 -20.419 1.00 0.37 1991242
	ATOM 1244 001	24.001 59.420 -21.283 1.00 0.37 1sG1244
	ATOM 1245 CG2 THR 152	23.764 60.239 -20.631 1.00 0.37 ISG1245
	ATOM 1246 C THR 152	25.993 57 273 -21 235 1 00 0.37 ISG1246
45	ATOM 1240 M	27.222 57.258 -21.206 1.00 0.37
		25.276 56.407 -21.972 1.00 0.21 1861240
	3 move 1000	24 927 54 865 22 622 1.00 0.21 1SG1250
	ATOM 1251 0 GLY 153	23.727 54 978 -23 440 1.00 0.21 ISG1251
50	ATOM 1252 N LYS 154 2	25.384 54 221 -24 701 1 00 0.21 ISG1252
50		24.429 53.670 -25.687 1.00 0 12 1561253
	3004 1005	4.681 54.054 -27.152 1.00 0 12 1501255
	BTOM 1956 on The	5 103 55 076 22 774 14 1.00 0.12 1SG1256
EE	ATOM 1257 CE LYS 154 2	4.981 57 477 20 040 1.00 U.12 1SG1257
55	ATOM 1258 NZ LYS 154 2	5.536 57 901 30 200 1.00 0.12 1SG1258
		4.520 52.188 -25.611 1.00 0 12 1501260
	ATOM 1261 W	5.575 51.600 -25.848 1.00 0.12 1901261
	3 move 1000 m	3.395 51.548 -25.250 1.00 0.20 1SG1262
60	ATOM 1263 CB VAL 155 2:	2.778 49 535 23 005 1.00 0.20 ISG1263
	ATOM 1264 CG1 VAL 155 25	3.730 49.874 -22.924 1.00 0.20 ISG1264
	ATOM 1265 CG2 VAL 155 21	1.347 50.064 -23.790 1.00 0.20 1991266
		2.424 49.793 -26.367 1.00 0.20 1551267
65	ATTOM 1260 W	1.364 50.401 -26.514 1.00 0.20 1SG1268
	ATOM 1269 CA TRP 156 21	3.830 48.847 -27.226 1.00 0.33 1SG1269
	ATOM 1270 CB TRP 156 20	1.541 49 207 27 040 1.00 0.33 ISG12/0
	ATOM 1271 CG TRP 156 20	0.416 46.980 -27.065 1.00 0.33 1SG1271
70		.349 45.628 -27.548 1.00 0.33 1861272
	3.00M 1074 seed	.351 46.905 -25.705 1.00 0.33 1SG1274
	100 ZU	.250 45.593 -25.308 1.00 0.33 1SG1275

	ATOM	1275 CI	22 TDD	156	20.04					
	ATOM	1276 CI		156	20.24 20.37		95 -26.43	33 1.0		1 SG 1276
	ATOM	1277 C	2 TRP	156	20.16	O 43.17	22 -28.81 38 -26.57	16 1.0		1 SG 1277
_	ATOM	1278 C	3 TRP	156	20.29		52 -28.94	70 1.0		1SG1278
5	ATOM	1279 CF	12 TRP	156	20.19		26 -27.84	19 1.0 18 1.0		15G1279
	MOTA	1280 C	TRP	156	21.97		7 -29.13	9 1.0		1SG1280
	ATOM	1281 0	TRP	156	22.91	6 50.59	5 -29.10	1.0		1SG1281 1SG1282
	MOTA	1282 N	GLN	157	20.88	0 50.01	4 - 29.89	2 1.0		15G1282
10	MOTA MOTA	1283 CA		157	20.74	2 51.17	8 -30.71	1 1.0		15G1284
	ATOM	1284 CB 1285 CG		157	19.49	1 51.11	4 -31.59	9 1.0	0 0.49	1SG1285
	ATOM	1286 CD		157 157	19.42		6 -32.44	7 1.0		1SG1286
	ATOM	1287 OE		157	20.71	49./4	4 -33.22	7 1.0		1SG1287
	ATOM	1288 NE		157	21.35		9 -33.85 7 -33.18	1 1.0		1 SG 1288
15	MOTA	1289 C	GLN	157	20.57	52 38	7 -33.18 2 -29.84			1SG1289
	MOTA	1290 O	GLN	157	21.157		3 -30.09	2 1.00 7 1.00		1SG1290
	ATOM	1291 N	LEU	158	19.769		2 -28.76	9 1.00		1SG1291
	ATOM	1292 CA	LEU	158	19.383	53.372	2 -27.97	1.00		1SG1292
20	ATOM	1293 CB	LEU	158	18.139	53.117	7 -27.10	5 1.00		1 SG1 293 1SG1294
2.0	MOTA	1294 CG	LEU	158	16.869	52.845	5 -27.933	3 1.00		1SG1295
	ATOM ATOM	1295 CD2	LEU	158	17.020	51.571	L -28.782	2 1.00		1SG1296
	ATOM	1296 CD1 1297 C		158	16.466	54.076	6 -28.762	2 1.00		1SG1297
	ATOM	1298 0		158 158	20.476	53.827	7 -27.067	1.00	0.41	1SG1298
25	ATOM	1299 N		159	21.433	53.107	-26.787	1.00		1SG1299
	ATOM	1300 CA		159	20.333	55 701	-26.610	1.00		1SG1300
	MOTA	1301 CB		159	21.643	57 142	-25.689 -26.138			1SG1301
		1302 CG	ASP	159	22.711	57.750	-25.227	1.00		1SG1302
20	ATOM	1303 OD1	ASP :	1 5 9	22.869	57.289	-24.067	1.00	0.19 0.19	1SG1303
30		1304 OD2		159	23.385	58.706	-25.697	1.00	0.19	1SG1304 1SG1305
		1305 C		159	20.460	55.850	-24.413	1.00	0.19	1SG1305
		1306 O 1307 N		159	19.280	56.200	-24.424	1.00	0.19	1SG1307
		1308 CA		160	21.100	55.535	-23.272	1.00	0.11	1SG1308
35		1309 CB		160 160	20.407	55.630	-22.022	1.00	0.11	1SG1309
		1310 CG		60	20.273	54.289	-21.280	1.00	0.11	1SG1310
		1311 CD1		.60	19.672	53.43/	-22.031 -23.207	1.00	0.11	1SG1311
	ATOM 1	1312 CD2	TYR 1	60	18.036	53.241	-23.207	1.00	0.11	1SG1312
4.0	ATOM 1	1313 CE1	TYR 1	.60	18.776	52.036	-23.892	1.00	0.11 0.11	1SG1313
40		1314 CE2		60	17.135	52.456	-22.225	1.00	0.11	1SG1314 1SG1315
		315 CZ		60	17.506	51.852	-23.402	1.00	0.11	1SG1316
		316 OH		60	16.587	51.045	-24.106	1.00	0.11	1SG1317
		.317 C .318 O		60	21.173	56.539	-21.122	1.00	0.11	1SG1318
45		319 N		60 61	22.366	56.770	-21.316	1.00	0.11	1SG1319
		320 CA		61	20.472 21.125	57.112	-20.124	1.00	0.12	1SG1320
		321 CB			20.623		-19.159	1.00	0.12	1 SG 1321
	ATOM 1	322 CG			21.484	60.299	-19.119	1.00	0.12	15G1322
F 0		323 CD	GLU 1		21.015	61.741	-18 382	1.00 1.00	0.12	1SG1323
50	ATOM 1	324 OE1	GLU 1		19.816	62.015	-18.112	1.00	0.12 0.12	1SG1324
		325 OE2			21.860	62.592	-18.773	1.00	0.12	1SG1325 1SG1326
			GLU 16		20.870	57.327	-17.824	1.00	0.12	1SG1327
			GLU 16		19.815	56.739	-17.589	1.00	0.12	1SG1328
55		`	SER 16		21.860	57.419	-16.919	1.00	0.11	1SG1329
			SER 16 SER 16		21.729	56.834 -	-15.619	1.00	0.11	1SG1330
			SER 16		23.065 22. 8 57	56.348 -	-15.030	1.00	0.11	1SG1331
			SER 16	_		55.774 - 57.852 -	14 600	1.00	0.11	1SG1332
60	ATOM 13		SER 16		1.083	59.035 -	-14.000	1.00	0.11	1SG1333
60		134 N (LU 16		0.754	57.391 -	13.012	1.00	0.11	15G1334
			LU 16		0.245	58.279 -	12.496		0.13 0.13	18G1335
			LU 16		9.399	57.559 -	11.433		0.13	1 SG 1336 1SG1337
		37 CG G	LU 16		0.166	56.464 -	10.691	1.00	0.13	15G1337
65	ATOM 13 ATOM 13	38 CD G	LU 16		9.148	55.604	-9. 9 57		0.13	1SG1339
	ATOM 13	39 OE1 G 40 OE2 G	LU 16	_	8.185	55.142 -	10.626		0.13	1SG1340
			LU 16: LU 16:			55.396	-8.726		0.13	1SG1341
			LU 16:		1.427 ! 2.501 !	58.899 -			0.13	1SG1342
7.0			RO 164		1.247	58.306 - 50.108 -	11 20E		0.13	1SG1343
70	ATOM 13		RO 164		2.340	50.787 -			0.13	1SG1344
	ATOM 13		RO 164		0.412	1.023 -	12.159		0.13 0.13	1SG1345
					-					1SG1346

	ATO	1 1346 0	B PR	164	21 00					
	ATON						1 -10.81	4 1.0	0 0.13	1SG1347
	ATON						3 -12.05		0 0.13	1SG1348
	ATOM	_								1SG1349
5	ATOM									1SG1350
	ATOM				24.14		•			1SG1351
	ATOM				25.04					1SG1352
	ATOM				24.39			-		1SG1353
	ATOM	1354 C	D2 LEU	165	22.95		-8.07			1SG1354
10	ATOM		ol LEU	165	25.27	56.226				1SG1355
	ATOM	1356 C	LEU		24.887					1SG1356
	ATOM		LEU	165	25.628					1SG1357
	ATOM		ASN	166	24.696		-5.65			1SG1358
15	ATOM				25.384		-5.06			1SG1359 1SG1360
10	ATOM				24.587	63.214	-3.980			15G1360 1SG1361
	ATOM ATOM	1361 CC		166	23.476		-4.64			1SG1362
	ATOM	1362 OI 1363 NI	ASN ASN	166	23.226		-5.845			1SG1363
	ATOM	1364 C			22.794		-3.846	1.00		15G1364
20	ATOM	1365 0	asn Asn	166	26.621		-4.414		0.10	1SG1365
	ATOM	1366 N	ILE	166 167	26.569		-3.537		0.10	1SG1366
	ATOM	1367 CA		167	27.780 29.021		-4.857			1SG1367
	ATOM	1368 CB		167	30.021		-4.261			1SG1368
	ATOM	1369 CG		167	31.364		-5.249			1SG1369
25	ATOM	1370 CG	1 ILE	167	29.500	61.380 60.285	-4.515			1SG1370
	ATOM	1371 CD	1 ILE	167	30.315	59.855	-5.918 -7.138	1.00		1SG1371
	ATOM	1372 C	ILE	167	29.588	63.326	-3.662			1SG1372
	ATOM	1373 o	ILE	167	29.637	64.372	-4.306		0.22	1SG1373
30	ATOM	1374 N	THR	168	30.016	63.251	-2.391	1.00	0.22 0.48	1SG1374
30	ATOM	1375 CA	THR	168	30.555	64.431	-1.790	1.00	0.48	1SG1375 1SG1376
	ATOM	1376 CB	THR	168	29.789	64.932	-0.603	1.00	0.48	1SG1376 1SG1377
	ATOM ATOM	1377 OG:		168	29.672	63.906	0.372	1.00	0.48	15G1378
	ATOM	1378 CG:		168	28.411	65.422	-1.054	1.00	0.48	1SG1379
35	ATOM	1380 0	THR THR	168	31.917	64.138	-1.288	1.00	0.48	1SG1380
	ATOM	1381 N	VAL	168 169	32.229	63.015	-0.894	1.00	0.48	1SG1381
	ATOM	1382 CA	VAL	169	32.784 34.061	65.163	-1.315	1.00	0.55	1SG1382
	ATOM	1383 CB	VAL	169	35.186	64.960 65.749	-0.722	1.00	0.55	15G1383
4.0	ATOM	1384 CG1	VAL	169	35.366	65.272	-1.338	1.00	0.55	1SG1384
40	ATOM	1385 CG2	VAL	169	34.903	67.254	-2.785 -1.220	1.00	0.55	1SG1385
	ATOM	1386 C	VAL	169	33.871	65.395	0.689	1.00 1.00	0.55	1SG1386
	ATOM	1387 o	VAL	169	33.425	66.509	0.960	1.00	0.55 0.55	15G1387
	ATOM	1388 N	ILE	170	34.178	64.492	1.631	1.00	0.56	1SG1388 1SG1389
45	ATOM	1389 CA	ILE	170	33.974	64.776	3.017	1.00	0.56	1SG1309
10	ATOM ATOM	1390 CB 1391 CG2	ILE	170	34.332	63.609	3.909	1.00	0.56	15G1391
		1391 CG2	ILE	170	35.849	63.375	3.822	1.00	0.56	1SG1392
	ATOM	1393 CD1	TIE	170	33.816	63.807	5.348	1.00	0.56	1SG1393
		1394 C	ILE	170 170	34.469	64.961	6.108	1.00	0.56	1SG1394
50		1395 0	ILE	170	34.831 34.414	65.949	3.356	1.00	0.56	1SG1395
		1396 N	LYS	171	36.052	66.833 65.993	4.103	1.00	0.56	1 SG 1396
	ATOM	1397 CA		171	36.958	67.069	2.792	1.00	0.52	1SG1397
		1398 СВ		171	38.241	66.953	3.063	1.00	0.52	15G1398
	ATOM	1399 CG		171	39.411	67.838	2.216 2.650	1.00	0.52	1SG1399
55		1400 CD		171	39.151	69.334	2.515	1.00	0.52	1SG1400
		1401 CE		171	40.396	70.193	2.745	1.00	0.52	1SG1401
		1402 NZ		171	40.985	69.879	4.064	1.00	0.52 0.52	15G1402
		1403 C		171		68.329	2.704	1.00	0.52	1SG1403 1SG1404
60		1404 0		171	35.772	68.490	1.578		0.52	15G1404 15G1405
00					36.106	69.253	3.677		0.31	1SG1405
						70.457	3.427		0.31	15G1407
						70.764	4.515	1.00	0.31	1SG1408
					36.321	71.645		1.00	0.31	1SG1409
65		410 OXT	ALA 1		35.863 37.507	72.767		1.00	0.31	1SG1410
	END			.,	-1.501	71.460	3.008	1.00	0.31	1SG1411

TABLE 4

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REMARK Model of the Fc Epsilon Receptor I 'dimer'; V.C. Epa, 28/08/98.

	ATOM ATOM	1 N VAL 2 CA VAL	A 1	l 35.03				
_	ATOM ATOM	3 C VAL. 4 O VAL.				7 -1.314	1.00 0.14	1 C
5	ATOM	5 CB VAL	A 1	37.48				
	ATOM ATOM	6 CG1 VAL 2 7 CG2 VAL 2	A 1 A 1				1.00 0.14	l c
	ATOM	8 1H VAL 1	A 1				1.00 0.14	
10	MOTA MOTA	9 2H VAL 1 10 3H VAL 1			1 67.268	-2.703	1.00 0.00	
	MOTA	11 HA VAL					1.00 0.00	
	ATOM ATOM	12 HB VAL A 13 1HG1 VAL A	1 1		1 67.089	-3.011	1.00 0.00	
1 0	ATOM	14 2HG1 VAL A	. 1		9 66.431 6 65.302		1.00 0.00 1.00 0.00	H
15	ATOM ATOM	15 3HG1 VAL A 16 1HG2 VAL A		36.46	3 66.547	-5.351	1.00 0.00 1.00 0.00	H H
	ATOM	17 2HG2 VAL A	. 1	38.22 36.57			1.00 0.00 1.00 0.00	H
	MOTA. MOTA	18 3HG2 VAL A 19 N PRO A		38.00	1 69.445	-3.249	1.00 0.00 1.00 0.00	H H
20	MOTA	20 CA PRO A		35.933 36.195			1.00 0.15 1.00 0.15	N
	ATOM ATOM	21 C PRO A 22 O PRO A	2	35.493	68.456		1.00 0.15 1.00 0.15	C
	ATOM	22 O PRO A 23 CB PRO A		34.546 35.731		0.973 0.391	1.00 0.15	0
25	MOTA ATOM	24 CG PRO A 25 CD PRO A	2	35.897	71.231	-1.067	1.00 0.15 1.00 0.15	c c
	ATOM	25 CD PRO A 26 HA PRO A	2 2	35.709 37.285		-1.884	1.00 0.15	С
	ATOM ATOM	27 1HB PRO A	2	36.304	71.370	0.558 1.118	1.00 0.00 1.00 0.00	H H
	ATOM	28 2HB PRO A 29 1HG PRO A	2 2	34.669 36.917		0.677	1.00 0.00	H
30	ATOM	30 2HG PRO A	2	35.203	72.033	-1.212 -1.366	1.00 0.00 1.00 0.00	H H
	ATOM ATOM	31 1HD PRO A 32 2HD PRO A	2 2	34.667 36.339	_	-2.239	1.00 0.00	H
	ATOM	33 N GLN A	3	35.941	70.042 68.473	-2.732 2.617	1.00 0.00 1.00 0.19	H N
35	ATOM ATOM	34 CA GLNA 35 C GLNA	3 3	35.329	67.651	3.614	1.00 0.19	C
	ATOM	36 O GLN A	3	33.901 33.553	68.073 69.196	3.703 3.339	1.00 0.19 1.00 0.19	C
	MOTA MOTA	37 CB GLN A 38 CG GLN A	3 3	35.986	67.803	4.996	1.00 0.19	o c
40	ATOM	39 CD GLN A	3	35.493 36.327	66.802 67.022	6.040 7.293	1.00 0.19 1.00 0.19	C
40	ATOM ATOM	40 OE1 GLN A 41 NE2 GLN A	3	36.930	68.079	7.467	1.00 0.19 1.00 0.19	с 0
	MOTA	42 H GLN A	3 3	36.374 36.686	65.997 69.083		1.00 0.19 1.00 0.00	N
	atom Atom	43 HA GLNA 44 1HB GLNA	3	35.401	66.596	3.289	1.00 0.00 1.00 0.00	H H
45	MOTA	45 2HB GLN A	3 3	35.828 37.076	68.836 67.663		1.00 0.00 1.00 0.00	H
	ATOM ATOM	46 1HG GLN A 47 2HG GLN A	3	35.596	65.769	5.669	1.00 0.00 1.00 0.00	H H
	ATOM	48 1HE2 GLN A	3 3	34.444 36.281	66.987 65.050		1.00 0.00 1.00 0.00	H
50	ATOM ATOM	49 2HE2 GLN A 50 N LYS A	3	37.049	66.168		1.00 0.00 1.00 0.00	H H
	ATOM	51 CA LYS A	4 4	33.024 31.626	67.165 67.476		1.00 0.23 1.00 0.23	N
	ATOM ATOM	52 C LYS A 53 O LYS A	4	31.282	67.937		1.00 0.23 1.00 0.23	C C
	ATOM	53 O LYS A 54 CB LYS A	4 4	31.667 30.722	67.348 66.273		.00 0.23	0
55	ATOM ATOM	55 CG LYS A 56 CD LYS A	4	30.861	65.765		.00 0.23	C C
	ATOM	56 CD LYS A 57 CE LYS A	4	30.229 31.032	64.389 63.242		.00 0.23	С
	ATOM	58 NZ LYS A	4	30.320	61.959		.00 0.23	C N1+
60	ATOM ATOM	59 H LYS A 60 HA LYS A	4 4	33.282 31.442	66.218	4.377 1	.00 0.00	H
	ATOM	61 1HB LYS A	4	29.665	68.204 66.523		.00 0.00 .00 0.00	H H
	ATOM ATOM	62 2HB LYS A 63 1HG LYS A		30.952 31.919	65.468	4.623 1	.00 0.00	H
65	MOTA	64 2HG LYS A		30.360	65.737 66.486		.00 0.00 .00 0.00	H
0.5	ATOM ATOM	65 1HD LYS A 66 2HD LYS A			64.216	1.154 1	.00 0.00	H H
	ATOM	67 1HE LYS A	4		64.402 63.364		.00 0.00 .00 0.00	H
	ATOM ATOM	68 2HE LYS A 69 1HZ LYS A	4	32.027	63.149	2.391 1.	.00 0.00	H H
70	ATOM	69 1HZ LYS A 70 2HZ LYS A			61.167 61.981		00 0.00	H
	ATOM	71 3HZ LYS A	-		61.756	_	00 0.00	H H

	ATOM ATOM	73 CA		5	30.10	8 69.61				N C
5	ATOM ATOM ATOM	75 O	PRO A PRO A PRO A	5 5 5	29.27 28.73 29.23	0 67.71	9 6.83	22 1.00 39 1.00	0.25	С 0
	ATOM ATOM	77 CG 78 CD		5 5	28.59 29.67	2 70.25	7 5.11	2 1.00	0.25	0 0
10	MOTA MOTA	79 HA 80 1HB	PRO A	5 5	30.97 29.73	2 69.90 0 71.74	6 7.45	6 1.00	0.00	C H H
10	ATOM ATOM	81 2HB 82 1HG 83 2HG	PRO A PRO A PRO A	5 5 5	28.45 28.17 27.91	4 70.97	2 4.41	2 1.00	0.00	H
1 =	MOTA MOTA	84 1HD 85 2HD	PRO A	5	29.23	6 68.46	9 4.04	4 1.00	0.00 0.00 0.00	H
15	MOTA MOTA MOTA	86 N 87 CA	LYS A LYS A	6	29.172 28.33	68.639 67.689	9 8.86	1 1.00	0.35	H N C
	ATOM ATOM	88 C 89 O 90 CB	LYS A LYS A LYS A	6 6 6	27.209 27.391 29.033	69.53	10.66	6 1.00	0.35 0.35	С 0
20	MOTA MOTA	91 CG 92 CD	LYS A	6	30.016 31.243	65.843	10.12	7 1.00	0.35 0.35 0.35	0 0
	ATOM ATOM ATOM	93 CE 94 NZ 95 H	LYS A	6	32.218 33.370	65.365 66.010	8.920 8.253	1.00	0.35 0.35	C N1+
25	ATOM ATOM	96 HA 97 1HB	LYS A LYS A LYS A	6 6 6	29.530 27.947 28.241	66.943	8.805	1.00	0.00	H
	ATOM ATOM	98 2HB 99 1HG	LYS A LYS A	6 6	29.641 29.498		11.336	1.00	0.00 0.00 0.00	H H H
30	MOTA MOTA MOTA	100 2HG 101 1HD 102 2HD	LYS A LYS A LYS A	6 6	30.343 31.763 30.880	65.221 67.118	10.981 10.116	1.00	0.00 0.00	H H
	MOTA MOTA	103 1HE 104 2HE	LYS A	6	31.740 32.610	67.022 64.699 64.746	8.600 8.183 9.743	1.00	0.00 0.00 0.00	H H H
35	ATOM ATOM ATOM	105 1HZ 106 2HZ 107 3HZ	LYS A LYS A LYS A	6	33.989	65.352 66.644	7.805 7.532	1.00	0.00	H H
	ATOM ATOM	108 N	VAL A	6 7 7	33.939 25.995 24.871	66.555 67.867 68.517	8.889 10.051 10.651	1.00 1.00 1.00	0.00	H N
40	ATOM ATOM	111 0	VAL A VAL A	7	24.592 24.524	67.792 66.564	11.922 11.950	1.00	0.35 0.35 0.35	с с о
	ATOM ATOM ATOM	113 CG1	VAL A VAL A VAL A	7 7 7	23.627 23.210 22.552	68.483 67.019	9.806 9.585	1.00	0.35 0.35	C C
45	ATOM ATOM	115 H 116 HA	VAL A VAL A	7 7	25.821 25.120	69.335 66.977 69.575	10.499 9.615 10.831	1.00 1.00 1.00	0.35 0.00 0.00	С Н Н
	ATOM ATOM ATOM	117 HB 1 118 1HG1 1 119 2HG1 1	VAL A	7 7	23.863	68.941 66.965	8.827 8.765	1.00	0.00	H H
50	ATOM ATOM	120 3HG1 v 121 1HG2 v	VAL A	7 7 7	24.031 22.693 21.678	66.350 66.586 69.500	9.285		0.00	H
	ATOM ATOM	122 2HG2 V 123 3HG2 V	/AL A /AL A	7 7	22.176 22.944	68.844	9.847 11.412 10.791	1.00	0.00 0.00 0.00	H H H
55	ATOM ATOM ATOM	125 CA S	ER A	8 8 8	24.448	68.548 67.929	13.023 14.287	1.00	0.17 0.17	N C
	MOTA MOTA	127 o s	ER A	8 8	22.807 22.347 25.131	68.274 69.396 68.420	14.689 14.481 15.407	1.00	0.17 0.17 0.17	с о с
60	ATOM ATOM ATOM	130 H S	ER A		24.819 24.612	67.761 69.550	16.625 13.018	1.00	0.17	O
	ATOM ATOM	132 1HB S	ERA 6 ERA 6		24.337 25.070 26.175	66.838 69.509 68.173	14.216 15.536	1.00	0.00	H H
65	ATOM ATOM	134 HG S 135 N L	ERA 6 EUA 9	} } .	24.240	68.346 67.295	15.162 17.142 15.268	1.00 0	0.00 0.00 0.11	H H N
03	ATOM ATOM ATOM	137 C L	EUA 9 EUA 9 EUA 9)	20.747 20.696	67.539 67.369	15.682 17.164	1.00 0 1.00 0	.11	c c
7.0	MOTA MOTA	139 CB L	EUA 9 EUA 9 EUA 9) ;	19.749	66.532	17.700 15.080 15.512	1.00 0 1.00 0	.11 .11	0 C
70	ATOM ATOM	141 CD1 LE 142 CD2 LE	SUA 9	. :	17.732	68.081	14.988	1.00 0	.11 .11 .11	С С

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MOTA 143 H LEU A 22.476 66.399 15.518 1.00 0.00 MOTA 144 HA LEU A 20.438 9 68.549 15.382 1.00 0.00 MOTA 145 1HB LEU A 9 20.066 65.510 15.354 1.00 0.00 MOTA 146 2HB LEU A 9 19.815 66.582 13.978 5 1.00 0.00 MOTA 147 HG LEU A 9 18.324 66.981 16.546 1.00 0.00 ATOM 148 1HD1 LEU A 9 16.651 68.121 15.191 1.00 0.00 ATOM 149 2HD1 LEU A 9 18.211 68.929 15.488 1.00 0.00 ATOM 150 3HD1 LEU A 9 17.848 68.122 13.899 1.00 0.00 ATOM 151 16.368 17.440 1HD2 LEU A 9 65.690 15.400 10 1.00 0.00 ATOM 2HD2 LEU A 152 9 65.417 14.015 1.00 0.00 MOTA 153 3HD2 LEU A 9 17.775 64.610 15.558 0.00 1.00 ATOM 154 ASN A N 10 20.176 68.388 17.872 1.00 0.17 MOTA 155 CA ASN A 10 20.046 68.267 19.291 1.00 0.17 MOTA 156 С ASN A 10 18.653 68.686 19.623 15 1.00 0.17 MOTA 157 0 ASN A 10 18.240 69.797 19.295 1.00 0.17 ATOM 158 CB ASN A 10 20.992 69.194 20.070 1.00 0.17 ATOM 159 CG ASN A 10 22.415 68.721 19.819 1.00 0.17 MOTA OD1 ASN A 160 10 23.167 69.361 19.086 1.00 0.17 ATOM 161 ND2 ASN A 10 22.798 67.574 20.443 20 1.00 0.17 ATOM 162 Н ASN A 10 19.900 69.270 17.449 1.00 0.00 ATOM 163 HA ASN A 10 20.331 67.257 19.576 1.00 0.00 MOTA 164 1HB ASN A 10 20.746 69.138 21.144 1.00 0.00 MOTA 165 2HB ASN A 10 20.917 70.239 19.756 1.00 0.00 MOTA 166 1HD2 ASN A 10 22.193 67.061 25 21.052 1.00 0.00 H ATOM 167 2HD2 ASN A 10 23.732 67.251 20.255 1.00 0.00 ATOM н 168 N PRO A 11 17.897 67.828 20.245 1.00 0.35 N PRO A 11 MOTA 169 CA 18.370 66.510 20.559 1.00 0.35 C MOTA 170 PRO A С 11 18.404 65.700 19.305 1.00 0.35 MOTA C 171 PRO A 11 0 17.867 66.139 18.290 1.00 30 0.35 MOTA PRO A 11 172 CB 17.403 65.958 21.604 1.00 0.35 C ATOM 173 PRO A 11 CG 16.865 67.215 22.308 1.00 0.35 С ATOM 174 CD PRO A 11 16.938 68.307 21.228 1.00 0.35 MOTA С 175 PRO A 11 HA 19.324 66.603 21.103 1.00 0.00 H ATOM 17.862 176 1HB PRO A 11 65.215 22.273 35 1.00 0.00 H PRO A 11 ATOM 177 2HB 16.571 65.464 21.082 1.00 0.00 н ATOM 178 1HG PRO A 11 17.522 67.473 23.155 1.00 0.00 ATOM Н 179 PRO A 2HG 11 15.851 67.097 22.721 1.00 0.00 H ATOM 180 1HD PRO A 11 15.961 68.435 20.733 ATOM 1.00 0.00 H 181 2HD PRO A 11 17.234 69.288 21.626 40 1.00 0.00 H ATOM 182 N PRO A 12 19.030 64.557 19.364 1.00 0.52 N MOTA 183 CA PRO A 12 19.156 63.710 18.209 1.00 0.52 C MOTA 184 C PRO A 17.853 12 63.101 17.809 1.00 0.52 С ATOM 185 0 PRO A 12 17.789 62.501 16.737 1.00 0.52 ATOM 186 PRO A 12 CB 20.215 62.672 18.568 1.00 0.52 45 C ATOM 187 CG PRO A 12 21.088 63.386 19.613 1.00 0.52 C ATOM 188 CD PRO A 20.128 12 64.371 20.299 1.00 0.52 C MOTA 189 HA PRO A 12 19.493 64.305 17.344 1.00 0.00 Н PRO A 12 ATOM 190 1HB 20.766 62.306 17.688 1.00 0.00 H ATOM 191 2HB PRO A 12 19.733 61.793 19.029 1.00 50 0.00 H ATOM 192 1HG PRO A 12 21.889 63.941 19.096 1.00 PRO A 12 0.00 MOTA 193 2HG 21.583 20.323 62.706 1.00 0.00 Н ATOM 194 1HD PRO A 12 19.742 63.953 21.242 1.00 0.00 H MOTA 195 2HD PRO A 12 20.663 65.299 20.521 1.00 0.00 MOTA 196 N TRP A 13 16.809 63.231 18.646 55 1.00 0.35 N TRP A 13 MOTA 197 CA 15.559 62.588 18.359 1.00 0.35 C MOTA 198 TRP A С 13 15.107 63.016 16.998 1.00 0.35 C MOTA 199 0 TRP A 13 14.934 64.204 16.731 1.00 0.35 0 MOTA 200 TRP A 13 CB 14.454 62.959 19.361 1.00 0.35 C MOTA 201 CG TRP A 13 14.839 62.683 20.795 1.00 60 0.35 C MOTA 202 CD1 TRP A 13 14.961 63.559 21.833 1.00 0.35 С ATOM 203 CD2 TRP A 13 15.219 61.396 21.302 1.00 0.35 С MOTA 204 NE1 TRP A 13 15.382 62.897 22.961 1.00 0.35 N MOTA 205 CE2 TRP A 13 15.549 61.564 22.647 1.00 0.35 С ATOM 206 CE3 TRP A 13 15.297 60.175 20.695 1.00 65 0.35 ATOM CZ2 TRP A 207 13 15.962 60.510 23.408 1.00 0.35 C MOTA 208 CZ3 TRP A 13 15.707 59.110 21.468 1.00 0.35 C MOTA 209 TRP A CH2 13 16.031 59,276 22.798 1.00 0.35 C MOTA 210 H TRP A 13 16.881 63.779 19.484 1.00 0.00 H MOTA 211 HA TRP A 13 15.723 61.498 18.375 1.00 70 0.00 MOTA 212 1HB TRP A 13 13.543 62.407 19.077 1.00 0.00 H MOTA 213 2HB TRP A 13 14.206 64.025 19.251 1.00 0.00 H

	ATON		3 14.739 64.617	21.844 1.00	0.00 н
	ATOM ATOM		3 15.809 63.343 3 15.045 60.031	23.741 1.00	0.00 н
5	ATOM	217 HZ2 TRP A 1			0.00 H
J	ATOM ATOM		3 15.795 58.114	21.062 1.00	0.00 H
	ATOM				0.00 H
	ATOM	221 CA ASN A 1	4 14.506 62.327	16.085 1.00 14.747 1.00	0.15 N 0.15 C
10	ATOM ATOM			14.777 1.00	0.15 C
	ATOM	224 CB ASN A 1		14.064 1.00 13.785 1.00	0.15 0
	ATOM ATOM		13.588 60.064	13.785 1.00 14.181 1.00	0.15 c 0.15 c
	ATOM	226 OD1 ASN A 16 227 ND2 ASN A 16		15.357 1.00	0.15 o
15	ATOM	228 H ASN A 14		13.165 1.00 16.292 1.00	0.15 N 0.00 H
	MOTA MOTA	229 HA ASN A 14 230 1HB ASN A 14	15.111 63.154	14.342 1.00	0.00 H
	ATOM	230 1HB ASN A 14 231 2HB ASN A 14		13.806 1.00	0.00 H
20	ATOM	232 1HD2 ASN A 14	12.990 59.778	12.763 1.00 12.202 1.00	0.00 H 0.00 H
20	MOTA MOTA	233 2HD2 ASN A 14 234 N ARG A 15		13.379 1.00	0.00 н
	ATOM	235 CA ARG A 15		15.615 1.00 15.668 1.00	0.13 N
	ATOM ATOM	236 C ARG A 15	10.645 63.247	15.668 1.00 16.872 1.00	0.13 C 0.13 C
25	ATOM	237 O ARG A 15 238 CB ARG A 15	11.086 62.908 9.961 61.164	17.969 1.00	0.13
	ATOM	239 CG ARG A 15	9.961 61.164 9.990 60.171	15.860 1.00 14.698 1.00	0.13 C
	ATOM ATOM	240 CD ARG A 15 241 NE ARG A 15	9.087 58.956	14.925 1.00	0.13 C 0.13 C
	ATOM	241 NE ARG A 15 242 CZ ARG A 15	9.233 58.061 8.137 57.682	13.742 1.00	0.13 N1+
30	ATOM	243 NH1 ARG A 15	8.137 57.682 6.892 58.097	13.023 1.00 13.396 1.00	0.13 C 0.13 N
	ATOM ATOM	244 NH2 ARG A 15 245 H ARG A 15	8.289 56.882	11.926 1.00	0.13 N 0.13 N
	ATOM	245 H ARG A 15 246 HA ARG A 15	12.592 61.259 10.563 62.903	4 4 5 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	0.00 н
35	ATOM	247 1HB ARG A 15	8.996 61.516		0.00 н 0.00 н
33	ATOM ATOM	248 2HB ARG A 15 249 1HG ARG A 15	10.355 60.612	4.6 555	0.00 н 0.00 н
	ATOM	249 1HG ARG A 15 250 2HG ARG A 15	11.007 59.776 9.785 60.645	40 maa	0.00 н
	ATOM ATOM	251 1HD ARG A 15	8.048 59.228	15.153 1.00	0.00 н 0.00 н
40	ATOM	252 2HD ARG A 15 253 HE ARG A 15	9.459 58.433	15.807 1.00	0.00 н
	ATOM	254 1HH1 ARG A 15	C 210		0.00 н 0.00 н
	ATOM ATOM	255 2HH1 ARG A 15 256 1HH2 ARG A 15	6.069 57.748	12.956 1.00 ().00 H).00 H
	ATOM	256 1HH2 ARG A 15 257 2HH2 ARG A 15			.00 н
45	ATOM	258 N ILE A 16).00 H).12 N
	atom Atom	259 CA ILE A 16 260 C ILE A 16	9.719 65.221	17.838 1.00 0	.12 C
	ATOM	261 O ILE A 16			.12 C
50	ATOM ATOM	262 CB ILE A 16	10.558 66.467		.12 o .12 c
	ATOM	263 CG1 ILE A 16 264 CG2 ILE A 16	10.236 67.383 1	16.690 1.00 0	.12 C
	ATOM	265 CD1 ILE A 16			.12 C
	ATOM ATOM	266 H ILE A 16 267 HA ILE A 16	9.590 64.694 1	5.804 1.00 0	.00 н
5 5	ATOM	268 HB ILE A 16	10 202		.00 н
	ATOM	269 1HG1 ILE A 16			.00 н .00 н
	ATOM ATOM	270 2HG1 ILE A 16 271 1HG2 ILE A 16	10.633 66.927 1	5.766 1.00 0.	.00 н
	ATOM	272 2HG2 ILE A 16			.00 н
60	ATOM	273 3HG2 ILE A 16	12.376 65.543 1		.00 н .00 н
	ATOM ATOM	274 1HD1 ILE A 16 275 2HD1 ILE A 16	10.934 69.273 1	5.860 1.00 0.	00 н
	ATOM	275 2HD1 ILE A 16 276 3HD1 ILE A 16			00 H
65	ATOM ATOM	277 N PHE A 17	7.862 66.360 18		00 H 17 N
	ATOM	278 CA PHE A 17 279 C PHE A 17	6.527 66.870 18	.904 1.00 0.	17 C
	ATOM	280 O PHE A 17	6.595 68.309 18 7.645 68.943 18		17 c
	ATOM ATOM	281 CB PHE A 17	5.886 66.867 20	3.627 1.00 0.).300 1.00 0.	
70	ATOM	282 CG PHE A 17 283 CD1 PHE A 17	5.562 65.480 20	.720 1.00 0.	17 C
	ATOM	284 CD2 PHE A 17		192 1.00 0. 657 1.00 0.	

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ATOM 285 CE1 PHE A 17 4.154 63.561 20.585 1.00 0.17 C ATOM 286 CE2 PHE A 17 6.027 63.563 22.057 1.00 0.17 ATOM 287 CZ PHE A 17 4.935 62.927 21.518 1.00 0.17 С MOTA 288 PHE A H 17 8.468 66.690 19.582 1.00 5 0.00 ATOM H 289 HA PHE A 17 5.913 66.277 18.229 1.00 0.00 H ATOM 290 1HB PHE A 17 4.946 67.418 20.184 1.00 0.00 H ATOM 291 2HB PHE A 17 6.495 67.400 21.041 1.00 0.00 H MOTA 292 HD1 PHE A 17 3.883 65.351 19.440 1.00 0.00 H MOTA 293 HD2 PHE A 17 7.205 65.348 22.059 1.00 0.00 10 ATOM H 294 HE1 PHE A 17 3.235 63.140 20.300 1.00 0.00 MOTA 295 HE2 PHE A 17 6.677 63.097 22.778 1.00 0.00 H MOTA 296 HZPHE A 17 4.352 62.236 22.047 1.00 0.00 H MOTA 297 N LYS A 18 5.446 68.858 18.119 1.00 0.22 N MOTA 298 CA LYS A 18 5.403 70.243 17.781 15 1.00 0.22 C MOTA 299 C LYS A 18 5.558 70.999 19.056 1.00 0.22 C MOTA 300 LYS A 0 18 5.134 70.546 20.119 1.00 0.22 0 ATOM 301 CB LYS A 18 4.077 70.663 17.126 1.00 0.22 C ATOM 302 CG LYS A 18 2.859 70.405 18.012 1.00 0.22 С ATOM 303 LYS A CD 18 1.586 71.086 17.511 1.00 20 0.22 C ATOM 304 CE LYS A 18 0.375 70.870 18.418 1.00 0.22 C MOTA 305 -0.743 NZ LYS A 18 71.728 17.967 1.00 0.22 N1+ ATOM 306 H LYS A 18 4.641 68.278 17.925 1.00 0.00 H ATOM 307 HA LYS A 18 6.267 70.377 17.128 1.00 0.00 ATOM H 308 1HB LYS A 18 3.964 70.148 25 16.156 1.00 0.00 H ATOM 309 2HB LYS A 18 4.150 71.742 16.902 1.00 0.00 ATOM H LYS A 310 1HG 18 3.038 70.808 19.019 1.00 0.00 ATOM 311 2HG LYS A 18 2.689 69.320 18.128 1.00 0.00 H ATOM 312 1HD LYS A 18 1.354 70.729 16.492 1.00 0.00 ATOM H 313 2HD LYS A 18 1.792 72.168 17,428 1.00 30 0.00 ATOM H 314 1HE LYS A 18 0.596 71.147 19.461 1.00 0.00 H ATOM 315 2HE LYS A 18 0.024 69.828 18.411 1.00 0.00 H ATOM 316 1HZ LYS A 18 -1.576 71.594 18.528 1.00 0.00 H MOTA 317 2HZ 72.713 71.517 LYS A 18 -0.522 18.013 1.00 0.00 MOTA H 318 3HZ LYS A 18 -1.016 17.014 1.00 35 0.00 Н MOTA 319 N GLY A 19 6.207 72.174 18.978 1.00 0.21 N ATOM 320 CA GLY A 19 6.383 72.980 20.146 1.00 0.21 MOTA 321 C С GLY A 19 7.708 72.652 20.746 1.00 0.21 C ATOM 322 0 GLY A 19 8.192 73.365 21.623 1.00 0.21 0 ATOM 323 H GLY A 19 6.494 72.539 18.071 1.00 40 0.00 ATOM 324 1HA GLY A 19 5.676 72.621 20.917 1.00 0.00 Н ATOM 325 2HA GLY A 19 6.080 74.028 20.096 1.00 0.00 ATOM H 326 N GLU A 20 8.338 71.560 20.281 1.00 0.23 N MOTA 327 CA GLU A 20 9.610 71.201 20.830 1.00 0.23 ATOM 328 GLU A 20 С 10.642 72.074 20.202 1.00 0.23 45 C ATOM 329 Ω GLU A 20 10.428 72.635 19.128 1.00 0.23 0 ATOM 330 CB GLU A 20 10.002 69.736 20.574 1.00 0.23 С ATOM 331 CG GLU A 20 9.106 68.753 21.327 1.00 0.23 C MOTA GLU A 332 CD 20 9.228 69.092 22.806 1.00 0.23 С ATOM 333 OE1 GLU A 20 10.378 69.332 23.263 1.00 0.23 50 0 ATOM 334 OE2 GLU A 20 8.174 69.131 23.495 1.00 0.23 01 ATOM 335 GLU A H 20 7.903 70.908 19.641 1.00 0.00 H ATOM 336 HA GLU A 20 9.596 71,403 21.915 1.00 0.00 ATOM H 337 1HB GLU A 20 11.054 69.593 20.883 1.00 0.00 H ATOM 338 2HB GLU A 9.998 20 69.547 19.493 55 1.00 0.00 H 339 1HG ATOM GLU A 20 9.443 67.718 21.165 1.00 0.00 H ATOM 340 2HG GLU A 20 8.053 68.826 21.031 1.00 0.00 H ATOM 341 N ASN A 21 11.794 72.224 20.879 1.00 0.16 N ATOM 342 CA ASN A 21 12.833 73.051 20.346 1.00 0.16 ATOM 343 С ASN A 21 13.814 72.151 19.677 1.00 0.16 60 C MOTA 344 0 ASN A 21 14.134 71.074 20.179 1.00 0.16 O MOTA 345 CB ASN A 21 13.589 73.859 21.415 1.00 0.16 C MOTA ASN A 346 CG 21 12.613 74.885 21.970 1.00 0.16 C ATOM 347 OD1 ASN A 21 11.595 75.174 21.347 1.00 0.16 0 MOTA ND2 ASN A 348 21 12.923 75.448 23.168 1.00 0.16 65 N MOTA 349 H ASN A 21 12.004 71.689 21.705 1.00 0.00 Н ATOM 350 HA ASN A 21 12.376 73.724 19.624 1.00 0.00 ATOM 351 1HB ASN A 21 14.424 74.395 20.932 1.00 0.00 H ATOM 352 2HB ASN A 21 13.999 73.200 22.196 1.00 0.00 Н ATOM 353 1HD2 ASN A 21 13.738 75.183 23.688 1.00 0.00 70 H ATOM 354 2HD2 ASN A 21 12.260 76.106 23.540 1.00 0.00 H ATOM 355 N VAL A 22 14.289 72.567 18.490 1.00 0.07

5	ATON ATON ATON ATON ATON ATON	13.77 C VALA 22 16.438 72.632 17.559 1.00 0.07 C 15.891 70.592 15.710 1.00 0.07 C 15.891 70.487 16.626 1.00 0.00 T 15.891 70.487 16.626 1.00 0.00 T 15.891 70.487 16.626 16.00 T 15.891 70.487 16.891 70.487 16.626 16.00 T 15.891 70.0
10	ATOM ATOM ATOM ATOM ATOM	363 HA VAL A 22 15.511 70.880 18.125 1.00 0.00 H 364 HB VAL A 22 14.492 72.177 15.798 1.00 0.00 H 365 1HG1 VAL A 22 15.529 70.095 14.795 1.00 0.00 H 366 2HG1 VAL A 22 16.697 71.275 15.398 1.00 0.00 H
15	ATOM ATOM ATOM ATOM ATOM	368 1HG2 VAL A 22 13.124 70.080 15.667 1.00 0.00 H 369 2HG2 VAL A 22 13.699 69.636 17.292 1.00 0.00 H 370 3HG2 VAL A 22 12.657 71.073 17.064 1.00 0.00 H 371 N THR A 23 17.641 72.066 17.762 1.00 0.00 H
20	ATOM ATOM ATOM ATOM	373 C THR A 23 18.823 72.838 17.530 1.00 0.06 C 374 O THR A 23 19.615 72.126 16.486 1.00 0.06 C 375 CB THR A 23 19.909 70.939 16.612 1.00 0.06 O 376 OG1 THR A 23 18.992 73.612 18.737 1.00 0.06 C
25	ATOM ATOM ATOM ATOM ATOM	378 H THR A 23 17.775 71.115 18.098 1.00 0.06 C 379 HA THR A 23 18.556 73.850 17.211 1.00 0.00 H 380 HB THR A 23 20.031 71.986 19.091 1.00 0.00 H 381 HG1 THR A 23 18.059 73.402 19.091 1.00 0.00 H
30	ATOM ATOM ATOM ATOM ATOM	382 1HG2 THR A 23 21.551 74.025 19.243 1.00 0.00 H 383 2HG2 THR A 23 21.585 73.297 17.628 1.00 0.00 H 384 3HG2 THR A 23 20.634 74.784 17.926 1.00 0.00 H 385 N LEU A 24 19.967 72.846 15.407 1.00 0.06 N
35	ATOM ATOM ATOM ATOM ATOM	388 O LEU A 24 22.058 72.966 14.393 1.00 0.06 C 389 CB LEU A 24 22.104 74.195 14.388 1.00 0.06 O 390 CG LEU A 24 20.163 72.461 12.965 1.00 0.06 C
40	ATOM ATOM ATOM ATOM ATOM	392 CD2 LEU A 24 18.814 70.318 13.167 1.00 0.06 C 393 H LEU A 24 19.688 73.815 15.281 1.00 0.00 H 394 HA LEU A 24 20.869 71.185 14.552 1.00 0.00 H 395 1HB LEU A 24 20.876 72.019 12.246 1.00 0.00 H
45	ATOM ATOM ATOM ATOM ATOM	397 HG LEU A 24 18.071 72.302 13.461 1.00 0.00 H 398 1HD1 LEU A 24 17.231 71.624 11.245 1.00 0.00 H 399 2HD1 LEU A 24 18.193 73.115 11.117 1.00 0.00 H 400 3HD1 LEU A 24 18.893 71.560 10.600 1.00 0.00 H
50	ATOM ATOM ATOM ATOM	402 2HD2 LEU A 24 17.820 69.888 12.973 1.00 0.00 H 403 3HD2 LEU A 24 19.551 69.756 12.571 1.00 0.00 H 404 N THR A 25 23.167 72.207 14.441 1.00 0.28 N
55	ATOM ATOM ATOM ATOM ATOM	406 C THR A 25 25.210 72.309 13.308 1.00 0.28 C 407 O THR A 25 25.220 71.106 13.059 1.00 0.28 C 408 CB THR A 25 25.235 72.590 15.697 1.00 0.28 C 409 OG1 THR A 25 24.523 73.038 16.841 1.00 0.28 C
60	ATOM ATOM ATOM ATOM ATOM	411 H THR A 25 23.130 71.194 14.477 1.00 0.00 H 412 HA THR A 25 24.322 73.946 14.351 1.00 0.00 H 413 HB THR A 25 25.413 71.521 15.855 1.00 0.00 H 414 HG1 THR A 25 24.344 73.978 16.692 1.00 0.00 H
	ATOM ATOM ATOM ATOM	416 2HG2 THR A 25 27.114 73.289 16.552 1.00 0.00 H 417 3HG2 THR A 25 27.249 72.875 14.839 1.00 0.00 H 418 N CYS A 26 25.878 73.197 12.565 1.00 0.52 N
65		420 C CYS A 26 28.050 72.983 11.446 1.00 0.52 C 421 O CYS A 26 28.460 74.132 11.908 1.00 0.52 C 422 CB CYS A 26 26.230 73.510 10.198 1.00 0.52 C 423 SG CYS A 26 27.098 72.999 8.709 1.00 0.52 C
70	MOTA	424 H CYS A 26 25.870 74.196 12.727 1.00 0.00 H 425 HA CYS A 26 26.399 71.671 11.235 1.00 0.00 H 426 1HB CYS A 26 26.355 74.595 10.346 1.00 0.00 H

	MOTA MOTA			6 25.17			1.00 0.00) н
	ATOM	428 N 429 CA		28.85 7 30.23				5 N
_	ATOM	430 C	_	7 31.04				
5	ATOM	431 0		7 30.62			1.00 0.35	
	ATOM	432 CB		7 30.71	3 71.117		1.00 0.35	
	ATOM	433 CG		7 30.59		12.743	1.00 0.35	
	ATOM ATOM		ASN A 2			12.228	1.00 0.35	
10	ATOM	436 H	ASN A 2 ASN A 2	_		12.855	1.00 0.35	
	ATOM	437 HA	ASN A 2			11.685	1.00 0.00	
	ATOM	438 1HB	ASN A 2			12.532 14.180	1.00 0.00 1.00 0.00	
	MOTA	439 2HB	ASN A 2			13.557	1.00 0.00	H H
15	ATOM	440 1HD2	ASN A 2			13.317	1.00 0.00	н
10	ATOM ATOM	441 2HD2 442 N				12.575	1.00 0.00	н
	ATOM	443 CA	GLY A 2			10.876	1.00 0.15	N
	ATOM	444 C	GLY A 2			9.762	1.00 0.15	C
0.0	ATOM	445 O	GLY A 28			9.623 10.382	1.00 0.15 1.00 0.15	C
20	ATOM	446 H	GLY A 28			11.502	1.00 0.15 1.00 0.00	о н
	ATOM	447 1HA	GLY A 28			8.837	1.00 0.00	н
	MOTA MOTA	448 2HA 449 N	GLY A 28		71.234	9.918	1.00 0.00	Н
	ATOM		ASN A 29 ASN A 29			8.633	1.00 0.16	N
25	ATOM		ASN A 29			8.454	1.00 0.16	С
	ATOM		ASN A 29			8.021 7.315	1.00 0.16 1.00 0.16	C
	ATOM		ASN A 29			7.382	1.00 0.16 1.00 0.16	o C
	ATOM		ASN A 29		73.331	7.919	1.00 0.16	č
30	ATOM ATOM		ASN A 29			9.096	1.00 0.16	ŏ
30	ATOM		ASN A 29			7.029	1.00 0.16	N
	ATOM		ASN A 29 ASN A 29	35.005 36.207		8.013	1.00 0.00	H
	ATOM		ASN A 29	37.363	74.723 75.225	9.419 7.240	1.00 0.00	H
2.5	ATOM	460 2HB	ASN A 29	36.417	73.884	6.449	1.00 0.00 1.00 0.00	H
35	ATOM	461 1HD2	ASN A 29	38.833	73.235	6.078	1.00 0.00	н н
	ATOM	462 2HD2 1		39.532	72.304	7.380	1.00 0.00	н
	ATOM ATOM		ASN A 30	35.187	76.815	8.463	1.00 0.16	N
	ATOM		ASN A 30 ASN A 30	34.377 35.268	77.945	8.127	1.00 0.16	С
40	ATOM		ASN A 30	36.420	79.043 79.153	7.645 8.060	1.00 0.16	C
	ATOM		ASN A 30	33.609	78.491	9.339	1.00 0.16 1.00 0.16	o C
	ATOM		ASN A 30	32.795	79.688	8.886	1.00 0.16	C
	ATOM ATOM	469 OD1 A 470 ND2 A		32.210	79.707	7.805	1.00 0.16	ŏ
45	ATOM		LSN A 30 LSN A 30	32.781	80.740		1.00 0.16	N
	ATOM		SN A 30	36.004 33.660	77.014		1.00 0.00	H
	ATOM		SN A 30	34.308	77.670 78.750		1.00 0.00 1.00 0.00	H
	MOTA	474 2HB A	SN A 30	32.904	77.733		1.00 0.00 1.00 0.00	H H
50	ATOM	475 1HD2 A	SN A 30	33.250	80.708		1.00 0.00	н
30	ATOM ATOM	476 2HD2 A 477 N P		32.054	81.435		1.00 0.00	H
	ATOM		HE A 31 HE A 31	34.745 35.486	79.879		1.00 0.12	N
	ATOM		HE A 31	35.228	81.003 82.101		1.00 0.12	С
	ATOM		HE A 31	34.243	82.101		1.00 0.12 1.00 0.12	C
55	ATOM		HE A 31	35.024	81.481		1.00 0.12 1.00 0.12	O C
	ATOM		HE A 31	35.870	82.641		1.00 0.12	č
	ATOM ATOM	483 CD1 P1		37.137	82.444		1.00 0.12	č
	ATOM	484 CD2 PI 485 CE1 PI		35.395	83.926		1.00 0.12	С
60	ATOM	486 CE2 PI		37.919 36.173	83.513 84.999		0.12	С
	ATOM		HE A 31	37.439	84.793		0.12	C
	ATOM	488 H PH	E A 31	33.732	79.978		.00 0.12	C H
	ATOM		IE A 31	36.560	80.758		.00 0.00	H
65	ATOM		IE A 31	33.955	81.746		.00 0.00	H
00	ATOM ATOM		IE A 31		80.664	4.121 1	.00 0.00	н
	ATOM	492 HD1 PH 493 HD2 PH			81.438		.00 0.00	H
	ATOM	494 HE1 PH			84.066		.00 0.00	H
7.0	ATOM	495 HE2 PH					.00 0.00	H
70	ATOM	496 HZ PH	E A 31				.00 0.00 .00 0.00	H
	ATOM	497 N PH	E A 32			_	.00 0.11	H N

	ATOM ATOM ATOM	499 C PHE A 500 O PHE A	32 35.851 84.13 32 34.911 85.10 32 35.322 86.08	4 7.598 1.	00 0.11 C 00 0.11 C 00 0.11 O
5	ATOM ATOM ATOM ATOM	502 CG PHE A 503 CD1 PHE A 504 CD2 PHE A	32 37.114 84.89 32 37.971 83.87 32 38.800 83.07 32 37.941 83.70	95 8.670 1. 75 9.336 1. 76 8.583 1.	00 0.11 C 00 0.11 C 00 0.11 C 00 0.11 C
10	ATOM ATOM ATOM ATOM ATOM	506 CE2 PHE A 507 CZ PHE A 508 H PHE A	32	7 9.178 1. 8 11.300 1. 7 10.542 1.	00 0.11 C 00 0.11 C 00 0.11 C
15	ATOM ATOM ATOM ATOM	510 1HB PHE A 511 2HB PHE A 512 HD1 PHE A	32 35.409 83.69 32 36.811 85.70 32 37.630 85.36 32 38.864 83.21	9 9.143 1.0 0 9.358 1.0 8 7.820 1.0 4 7.507 1.0	00 0.00 H 00 0.00 H 00 0.00 H
20	ATOM ATOM ATOM ATOM	514 HE1 PHE A 515 HE2 PHE A 516 HZ PHE A	32 37.287 84.32 32 40.252 81.50 32 38.705 82.63 32 40.190 81.21 33 33.600 84.83	8.572 1.0 2 12.380 1.0 7 11.019 1.0	00 0.00 H 00 0.00 H 00 0.00 H
	ATOM ATOM ATOM ATOM	518 CA GLU A 3 519 C GLU A 3 520 O GLU A 3	33.600 84.832 3 32.616 85.702 3 31.455 85.733 3 31.273 84.837 3 32.084 85.228	7.171 1.0 8.108 1.0 8.926 1.0	0 0.10 C 0 0.10 C 0 0.10 C
25	ATOM ATOM ATOM ATOM	522 CG GLU A 3 523 CD GLU A 3 524 OE1 GLU A 3 525 OE2 GLU A 3	3 31.401 83.860 3 30.934 83.526 3 30.393 84.442	5.863 1.0 4.456 1.0 3.782 1.0	0 0.10 C 0 0.10 C 0 0.10 C
30	ATOM ATOM ATOM ATOM	526 H GLUA 3 527 HA GLUA 3 528 1HB GLUA 3 529 2HB GLUA 3	3 33.268 83.963 3 33.037 86.717 3 32.872 85.275	8.132 1.0	0 0.00 H 0 0.00 H 0 0.00 H
35	ATOM ATOM ATOM ATOM ATOM	530 1HG GLU A 3 531 2HG GLU A 3 532 N VAL A 3 533 CA VAL A 3	30.550 83.937 32.063 83.066 30.644 86.808 29.511 86.925	6.545 1.00 6.242 1.00 8.020 1.00 8.884 1.00	0.00 H 0.00 H 0.09 N
40	ATOM ATOM ATOM ATOM	534 C VAL A 34 535 O VAL A 34 536 CB VAL A 34 537 CG1 VAL A 34 538 CG2 VAL A 34	28.077 85.132 28.792 88.229 27.594 88.260	8.570 1.00 9.470 1.00 8.712 1.00 9.674 1.00	0.09 C 0.09 O 0.09 C
45	ATOM ATOM ATOM ATOM	539 H VAL A 34 540 HA VAL A 34 541 HB VAL A 34	30.817 87.554 29.835 86.811 28.403 88.320	8.948 1.00 7.369 1.00 9.932 1.00 7.681 1.00	0.09 C 0.00 H 0.00 H
	ATOM ATOM ATOM ATOM	543 2HG1 VAL A 34 544 3HG1 VAL A 34 545 1HG2 VAL A 34	27.078 89.234 26.840 87.496 27.913 88.090 29.295 90.352	9.646 1.00 9.421 1.00 10.716 1.00 8.942 1.00	0.00 H 0.00 H 0.00 H 0.00 H
50	ATOM ATOM ATOM ATOM	546 2HG2 VAL A 34 547 3HG2 VAL A 34 548 N SER A 35 549 CA SER A 35 550 C SER A 35	30.288 89.266 30.583 89.418 28.277 85.587 27.364 84.531	9.931 1.00 8.177 1.00 7.274 1.00 6.942 1.00	0.00 H 0.00 H 0.11 N 0.11 C
55	ATOM ATOM ATOM ATOM	551 O SER A 35 552 CB SER A 35 553 OG SER A 35 554 H SER A 35	28.183 83.307 28.493 82.953 26.512 84.826 27.339 85.023 28.711 86.062	6.696 1.00 5.559 1.00 5.689 1.00 4.552 1.00	0.11 C 0.11 O 0.11 C 0.11 O
60	ATOM ATOM ATOM ATOM	555 HA SER A 35 556 1HB SER A 35 557 2HB SER A 35 558 HG SER A 35	28.711 86.062 26.653 84.371 25.922 85.742 25.812 83.985 27.975 84.275	6.500 1.00 7.771 1.00 5.827 1.00 5.528 1.00	0.00 H 0.00 H 0.00 H
65	ATOM ATOM ATOM ATOM	559 N SER A 36 560 CA SER A 36 561 C SER A 36 562 O SER A 36	28.548 82.623 29.398 81.472 28.707 80.338 29.282 79.676	4.528 1.00 7.794 1.00 7.742 1.00 7.057 1.00	0.00 H 0.27 N 0.27 C 0.27 C
7.0	ATOM ATOM ATOM ATOM	563 CB SER A 36 564 OG SER A 36 565 H SER A 36 566 HA SER A 36	29.776 80.977 30.410 82.020 28.273 82.996 30.311 81.701	6.194 1.00 9.147 1.00 9.871 1.00 8.696 1.00	0.27 O 0.27 C 0.27 O 0.00 H
70	ATOM ATOM	567 1HB SER A 36 568 2HB SER A 36	30.374 80.065 28.855 80.708	7.172 1.00 9.130 1.00 9.694 1.00	0.00 H 0.00 H

5	ATOM ATOM ATOM ATOM	70 N THR A 37 27.431 80.089 7.399 1.00 0.48 71 CA THR A 37 26.842 78.902 6.858 1.00 0.48 71 CA THR A 37 25.567 79.191 6.148 1.00 0.48	H N C
	ATOM ATOM ATOM ATOM ATOM	1 573 O THR A 37 24.911 80.206 6.377 1.00 0.48 1 574 CB THR A 37 26.522 77.882 7.901 1.00 0.48 1 575 OG1 THR A 37 25.965 76.737 7.283 1.00 0.48 1 576 CG2 THR A 37 25.515 78.485 8.896 1.00 0.48	0000
10	ATOM ATOM ATOM ATOM	578 HA THR A 37 27.513 78.421 6.132 1.00 0.00 579 HB THR A 37 27.418 77.638 8.460 1.00 0.00 580 HG1 THR A 37 25.715 76.122 7.988 1.00 0.00 581 1HG2 THR A 37 25.307 77.711 0.660	H H H H
15	MOTA MOTA MOTA MOTA MOTA	582 2HG2 THR A 37 25.923 79.370 9.399 1.00 0.00 1583 3HG2 THR A 37 24.557 78.741 8.418 1.00 0.00 1584 N LYS A 38 25.205 78.268 5.235 1.00 0.41 1585 CA LYS A 38 23.972 78.360 4.517 1.00 0.41	H H H N
20	ATOM MOTA ATOM MOTA	587 O LYS A 38 23.687 76.068 5.054 1.00 0.41 C 588 CB LYS A 38 24.131 78.210 2.995 1.00 0.41 C 589 CG LYS A 38 25.186 79.135 2.385 1.00 0.41 C 590 CD LYS A 38 26.617 79.135 2.385 1.00 0.41	
25	MOTA MOTA MOTA MOTA MOTA	591 CE LYS A 38 27.700 79.493 1.986 1.00 0.41 C 592 NZ LYS A 38 29.037 78.966 2.348 1.00 0.41 C 593 H LYS A 38 25.629 77.348 5.315 1.00 0.00 H 594 HA LYS A 38 23.477 79.318 4.738 1.00 0.00 H	1+
30	MOTA ATOM ATOM MOTA MOTA	596 2HB LYS A 38 24.408 77.173 2.761 1.00 0.00 H 597 1HG LYS A 38 24.996 80.183 2.681 1.00 0.00 H 598 2HG LYS A 38 25.082 79.106 1.285 1.00 0.00 H 599 1HD LYS A 38 26.726 77.658 2.649 1.00 0.00 H	
35	MOTA MOTA MOTA MOTA	601 1HE LYS A 38 27.684 80.565 2.244 1.00 0.00 H 602 2HE LYS A 38 27.598 79.398 0.893 1.00 0.00 H 603 1Hz LYS A 38 29.782 79.444 1.855 1.00 0.00 H 604 2Hz LYS A 38 29.227 79.092 3.336 1.00 0.00 H	
40	MOTA MOTA MOTA MOTA MOTA	605 3HZ LYS A 38 29.137 77.982 2.132 1.00 0.00 H 606 N TRP A 39 21.884 77.401 5.297 1.00 0.18 N 607 CA TRP A 39 21.073 76.294 5.707 1.00 0.18 C 609 O TRP A 39 19.565 77.005 4.659 1.00 0.18 C	
45	ATOM ATOM ATOM ATOM ATOM	610 CB TRP A 39 20.331 76.490 7.044 1.00 0.18 O 611 CG TRP A 39 21.211 76.379 8.268 1.00 0.18 C 612 CD1 TRP A 39 21.745 77.350 9.062 1.00 0.18 C 613 CD2 TRP A 39 21.658 75.123 8.802 1.00 0.18 C	
50	ATOM ATOM ATOM ATOM	615 CE2 TRP A 39 22.498 76.776 10.062 1.00 0.18 N 616 CE3 TRP A 39 22.453 75.405 9.912 1.00 0.18 C 617 CZ2 TRP A 39 21.425 73.840 8.397 1.00 0.18 C 618 CZ3 TRP A 39 23.031 74.401 10.636 1.00 0.18 C	
55	ATOM ATOM ATOM ATOM	619 CH2 TRP A 39 22.793 73.105 10.228 1.00 0.18 C 620 H TRP A 39 21.424 78.294 5.236 1.00 0.00 H 622 1HB TRP A 39 19.541 75.720 7.100 1.00 0.00 H	
	ATOM ATOM ATOM ATOM ATOM	623 2HB TRP A 39 19.802 77.454 7.048 1.00 0.00 H 624 HD1 TRP A 39 21.773 78.413 8.875 1.00 0.00 H 625 HE1 TRP A 39 23.073 77.294 10.699 1.00 0.00 H 626 HE3 TRP A 39 20.762 73.621 7.571 1.00 0.00 H	
60	ATOM ATOM ATOM ATOM	628 HZ3 TRP A 39 23.619 74.619 11.521 1.00 0.00 H 629 HH2 TRP A 39 21.828 71.796 8.843 1.00 0.00 H 630 N PHE A 40 19.690 74.803 4.416 1.00 0.08 N	
65	ATOM ATOM ATOM ATOM	632 C PHE A 40 17.664 73.654 4.057 1.00 0.08 C 633 O PHE A 40 17.990 72.739 4.811 1.00 0.08 O 634 CB PHE A 40 19.229 73.816 2.190 1.00 0.08 C 635 CG PHE A 40 20.153 74.766 1.514 1.00 0.08 C	
70	ATOM ATOM ATOM ATOM	636 CD1 PHE A 40 21.465 74.872 1.916 1.00 0.08 C 637 CD2 PHE A 40 19.703 75.553 0.478 1.00 0.08 C 638 CE1 PHE A 40 22.315 75.752 1.291 1.00 0.08 C 639 CE2 PHE A 40 20.551 76.435 -0.150 1.00 0.08 C	

	ATOM ATOM ATOM	641 H PHE A 40 20	0.105 74.013 4	257 1.00 0.08 C 892 1.00 0.00 H
5	MOTA MOTA MOTA	643 1HB PHE A 40 18 644 2HB PHE A 40 19 645 HD1 PHE A 40 21	3.376 73.555 1. 3.730 72.882 2.	136 1.00 0.00 H 549 1.00 0.00 H 471 1.00 0.00 H 717 1.00 0.00 H
10	MOTA MOTA MOTA	647 HE1 PHE A 40 23 648 HE2 PHE A 40 20	3.681 75.450 0. 3.355 75.778 1. 3.213 76.986 -1.	130 1.00 0.00 H 589 1.00 0.00 H 023 1.00 0.00 H
	MOTA MOTA MOTA MOTA	650 N HIS A 41 16 651 CA HIS A 41 15 652 C HIS A 41 14	3.383 73.945 3. 3.322 73.109 4. 620 72.643 3.	253 1.00 0.00 H 777 1.00 0.10 N 242 1.00 0.10 C 014 1.00 0.10 C
15	ATOM ATOM ATOM	654 CB HIS A 41 14 655 CG HIS A 41 13 656 ND1 HIS A 41 12	.287 73.836 5. .274 72.893 5. .236 73.278 6.	242 1.00 0.10 0 109 1.00 0.10 C 682 1.00 0.10 C 499 1.00 0.10 N
20	ATOM ATOM ATOM ATOM	658 CE1 HIS A 41 11 659 NE2 HIS A 41 12	.159 71.544 5. .548 72.151 6. .071 71.072 6.	541 1.00 0.10 C 310 1.00 0.10 C 253 1.00 0.10 N
25	MOTA MOTA MOTA MOTA	661 HA HIS A 41 15 662 1HB HIS A 41 13 663 2HB HIS A 41 14	.740 72.280 4.6 .796 74.642 4.5 .822 74.338 5.5	39 1.00 0.00 н
20	ATOM ATOM ATOM	665 HE1 HIS A 41 10. 666 HE2 HIS A 41 11. 667 N ASN A 42 14.	.744 70.826 5.0 .614 72.196 7.3 .764 70.142 6.4 .593 71.319 2.7	17 1.00 0.00 H 48 1.00 0.00 H 52 1.00 0.00 H
30	MOTA MOTA MOTA MOTA	668 CA ASN A 42 13. 669 C ASN A 42 14. 670 O ASN A 42 14.	.967 70.801 1.6 617 71.443 0.4 003 71.602 -0.6	22 1.00 0.11 C 40 1.00 0.11 C 14 1.00 0.11 O
35	MOTA MOTA MOTA	672 CG ASN A 42 11. 673 OD1 ASN A 42 12. 674 ND2 ASN A 42 10.	450 71.059 1.5 781 70.123 2.5 427 69.246 3.1 447 70.298 2.7	58 1.00 0.11 C 29 1.00 0.11 O
40	MOTA MOTA MOTA MOTA	675 H ASN A 42 14. 676 HA ASN A 42 14. 677 1HB ASN A 42 12. 678 2HB ASN A 42 12.	894 70.665 3.5 186 69.722 1.5 064 70.773 0.5	17 1.00 0.00 H 29 1.00 0.00 H 58 1.00 0.00 H
40	ATOM ATOM ATOM ATOM	679 1HD2 ASN A 42 9. 680 2HD2 ASN A 42 10. 681 N GLY A 43 15.	946 71.057 2.33 000 69.733 3.40 899 71.821 0.58	14 1.00 0.00 H 52 1.00 0.00 H 9 1.00 0.08 N
45	ATOM ATOM ATOM	683 C GLY A 43 16.3 684 O GLY A 43 16.6 685 H GLY A 43 16.2	364 73.848 -0.61 330 74.497 -1.54	1 1.00 0.08 c 6 1.00 0.08 0
50	ATOM ATOM ATOM ATOM	686 1HA GLY A 43 16.3 687 2HA GLY A 43 17.7 688 N SER A 44 15.6 689 CA SER A 44 15.3	323 71.897 -1.45 706 72.230 -0.37 517 74.428 0.34	8 1.00 0.00 H 4 1.00 0.00 H 6 1.00 0.15 N
	ATOM ATOM ATOM ATOM	690 C SER A 44 16.3 691 O SER A 44 16.5 692 CB SER A 44 13.9	45 76.510 1.16 13 76.111 2.31 64 76.262 0.69	7 1.00 0.15 C 7 1.00 0.15 O
55	ATOM ATOM ATOM	694 H SER A 44 15.0 695 HA SER A 44 15.4 696 1HB SER A 44 13.1	32 73.916 0.99 84 76.176 -0.78	0 1.00 0.15 O B 1.00 0.00 H
60	ATOM ATOM ATOM ATOM	697 2HB SER A 44 13.8 698 HG SER A 44 14.3 699 N LEU A 45 17.0	13 77.334 0.47 52 76.634 2.55 25 77.556 0.66	1.00 0.00 H 1.00 0.00 H 5 1.00 0.35 N
65	ATOM ATOM ATOM	701 C LEU A 45 17.29 702 O LEU A 45 16.19 703 CB LEU A 45 18.88	55 79.014 2.504 95 79.578 2.241	1.00 0.35 C 1.00 0.35 O
0.5	ATOM ATOM ATOM ATOM	704 CG LEU A 45 20.00 705 CD1 LEU A 45 20.84 706 CD2 LEU A 45 19.46 707 H LEU A 45 16.85	00 79.986 1.345 17 80.767 0.328 55 80.938 2.433	1.00 0.35 C 1.00 0.35 C 1.00 0.35 C
70	ATOM ATOM ATOM	708 HA LEU A 45 18.65 709 1HB LEU A 45 18.21 710 2HB LEU A 45 19.32	2 77.484 1.916 9 79.931 0.143	1.00 0.00 H 1.00 0.00 H 1.00 0.00 H 1.00 0.00 H

	ATOM ATOM ATOM	4 712 1HD1 LEU A 45 21.676 81.302 0.821 1.00 0.00 4 713 2HD1 LEU A 45 21.676 81.302 0.821 1.00 0.00	H H
5	MOTA MOTA MOTA MOTA	714 3HD1 LEU A 45 20.234 81.514 -0.203 1.00 0.00 715 1HD2 LEU A 45 19.719 81.980 2.158 1.00 0.00 716 2HD2 LEU A 45 18.389 81.005 2.576 1.00 0.00 717 3HD2 LEU A 45 20.074 80.759 3.311 1.00 0.00	H H H
10	ATOM ATOM ATOM ATOM	718 N SER A 46 17.808 79.040 3.734 1.00 0.48 719 CA SER A 46 17.218 79.785 4.809 1.00 0.48 720 C SER A 46 18.124 80.941 5.078 1.00 0.48 721 O SER A 46 19.320 80.771 5.301 1.00 0.48	HOCC
15	MOTA MOTA MOTA MOTA MOTA	722 CB SER A 46 17.159 79.037 6.154 1.00 0.48 723 OG SER A 46 16.268 77.937 6.093 1.00 0.48 724 H SER A 46 18.589 78.436 3.972 1.00 0.00 725 HA SER A 46 16.185 80.070 4.554 1.00 0.00	O C O H
20	ATOM ATOM ATOM ATOM	727 2HB SER A 46 18.133 78.779 6.591 1.00 0.00 17.728 HG SER A 46 16.014 77.771 7.023 1.00 0.00 17.729 N GLU A 47 17.561 82.158 5.029 1.00 0.44 17.730 CA GLU A 47 18.248 82.388 5.029 1.00 0.44	H H H N
2.5	MOTA MOTA MOTA MOTA	731 C GLU A 47 18.453 83.486 6.797 1.00 0.44 7 732 O GLU A 47 19.343 84.188 7.271 1.00 0.44 7 733 CB GLU A 47 17.440 84.622 4.906 1.00 0.44 7 734 CG GLU A 47 16.115 84.730 5.662 1.00 0.44	2
25	ATOM ATOM ATOM ATOM ATOM	735 CD GLU A 47 15.396 85.988 5.203 1.00 0.44 C 736 OE1 GLU A 47 15.858 86.606 4.206 1.00 0.44 C 737 OE2 GLU A 47 14.373 86.349 5.844 1.00 0.44 C 738 H GLU A 47 16.607 82.284 4.724 1.00 0.00 H	:))1-
30	ATOM ATOM ATOM ATOM ATOM	740 1HB GLU A 47 19.239 83.381 4.833 1.00 0.00 H 741 2HB GLU A 47 17.273 84.585 3.815 1.00 0.00 H 742 1HG GLU A 47 18.068 85.508 5.110 1.00 0.00 H 743 2HG GLU A 47 16.248 84.814 6.752 1.00 0.00 H	
35	ATOM ATOM ATOM ATOM	744 N GLU A 48 17.608 82.766 7.551 1.00 0.00 H 745 CA GLU A 48 17.419 82.881 8.969 1.00 0.45 N 746 C GLU A 48 18.648 82.740 9.823 1.00 0.45 C 747 O GLU A 48 18.857 82.570 1.823 1.00 0.45 C	
40	MOTA MOTA MOTA MOTA	748 CB GLU A 48 16.414 81.833 9.468 1.00 0.45 C 749 CG GLU A 48 16.862 80.403 9.154 1.00 0.45 C 750 CD GLU A 48 15.749 79.447 9.560 1.00 0.45 C 751 OE1 GLU A 48 14.717 79.838 10.837 1.00 0.45 C	
45	ATOM ATOM ATOM ATOM	752 OE2 GLU A 48 15.917 78.219 9.333 1.00 0.45 OI 753 H GLU A 48 16.949 82.175 7.075 1.00 0.00 H 755 1HB GLU A 48 15.437 82.052 8.999 1.00 0.00 H	
50	ATOM ATOM ATOM ATOM	756 2HB GLU A 48 16.290 81.972 10.557 1.00 0.00 H 757 1HG GLU A 48 17.655 80.150 9.869 1.00 0.00 H 758 2HG GLU A 48 17.413 80.258 8.238 1.00 0.00 H 759 N THR A 49 19.523 81.735 9.626 1.00 0.55 N	
	ATOM ATOM ATOM ATOM ATOM	760 CA THR A 49 20.475 81.591 10.695 1.00 0.55 C 761 C THR A 49 21.869 81.303 10.218 1.00 0.55 C 762 O THR A 49 22.124 81.078 9.036 1.00 0.55 O 763 CB THR A 49 20.062 80.467 11.603 1.00 0.55 C	
55	ATOM ATOM ATOM ATOM	765 CG2 THR A 49 20.139 79.164 10.795 1.00 0.55 C 766 H THR A 49 19.450 81.037 8.909 1.00 0.00 H 768 HB THR A 49 20.596 82.511 11.285 1.00 0.00 H	
60	ATOM ATOM ATOM ATOM	769 HG1 THR A 49 20.723 79.538 13.198 1.00 0.00 H 770 1HG2 THR A 49 19.326 78.450 10.800 1.00 0.00 H 771 2HG2 THR A 49 20.226 79.357 9.715 1.00 0.00 H 772 3HG2 THR A 49 21.061 78.660 1.100 0.00 H	
65	ATOM ATOM ATOM	773 N ASN A 50 22.808 81.331 11.191 1.00 0.44 N 774 CA ASN A 50 24.216 81.101 11.036 1.00 0.44 C 775 C ASN A 50 24.526 79.690 11.431 1.00 0.44 C 776 O ASN A 50 23.788 78.756 11.124 1.00 0.44	
70	ATOM ATOM ATOM ATOM ATOM	777 CB ASN A 50 25.082 82.012 11.923 1.00 0.44 C 778 CG ASN A 50 24.987 83.430 11.383 1.00 0.44 C 779 OD1 ASN A 50 25.306 83.682 10.223 1.00 0.44 O 780 ND2 ASN A 50 24.536 84.383 12.243 1.00 0.44 N 781 H ASN A 50 22.433 81.246 12.132 1.00 0.00 H	

5	ATON ATON ATON ATON ATON ATON	783 1HB ASN A 50 24.490 81.217 9.974 1.00 0.00 H 784 2HB ASN A 50 24.811 81.939 12.988 1.00 0.00 H 785 1HD2 ASN A 50 24.226 84.171 13.172 1.00 0.00 H 786 2HD2 ASN A 50 24.430 85.308 11.862 1.00 0.00 H	ł
10	MOTA MOTA MOTA MOTA MOTA	788 CA SER A 51 25.161 79.521 12.140 1.00 0.25 N 789 C SER A 51 25.171 77.448 13.267 1.00 0.25 C 790 O SER A 51 24.943 76.276 12.969 1.00 0.25 C 791 CB SER A 51 27.446 78.324 13.365 1.00 0.25 C 792 OG SER A 51 27.126 78.894 14.625 1.00 0.25 C	1
15	ATOM ATOM ATOM ATOM ATOM ATOM	794 HA SER A 51 26.417 77.665 11.581 1.00 0.00 H 795 1HB SER A 51 28.230 78.908 12.849 1.00 0.00 H 796 2HB SER A 51 27.829 77.295 13.499 1.00 0.00 H 797 HG SER A 51 27.896 78.769 15.200 1.00 0.00 H 798 N SER A 52 24.525 78.056 14.278 1.00 0.14 N	
20	MOTA MOTA ATOM MOTA MOTA	800 C SER A 52 22.214 77.760 14.740 1.00 0.14 C 801 O SER A 52 21.944 78.960 14.768 1.00 0.14 C 802 CB SER A 52 23.794 77.380 16.557 1.00 0.14 C 803 OG SER A 52 25.058 76.846 16.919 1.00 0.14 O 804 H SER A 52 23.794 77.380 16.557 1.00 0.14 C	
25	ATOM ATOM ATOM ATOM ATOM	805 HA SER A 52 23.703 76.203 14.814 1.00 0.00 H 806 1HB SER A 52 22.983 76.804 17.042 1.00 0.00 H 807 2HB SER A 52 23.706 78.429 16.892 1.00 0.00 H 808 HG SER A 52 25.161 76.977 17.872 1.00 0.00 H	
30	ATOM ATOM ATOM ATOM ATOM	810 CA LEU A 53 19.948 77.236 14.179 1.00 0.09 N 811 C LEU A 53 19.099 76.586 15.218 1.00 0.09 C 812 O LEU A 53 19.090 75.363 15.358 1.00 0.09 C 813 CB LEU A 53 19.400 76.833 12.798 1.00 0.09 C	
35	ATOM ATOM ATOM ATOM ATOM	815 CD1 LEU A 53 17.946 77.287 12.554 1.00 0.09 C 816 CD2 LEU A 53 17.822 78.817 12.594 1.00 0.09 C 817 H LEU A 53 21.500 75.830 14.376 1.00 0.00 H 818 HA LEU A 53 19.874 78.321 14.291 1.00 0.00 H	
40	ATOM ATOM ATOM ATOM ATOM	820 2HB LEU A 53 20.106 77.112 12.014 1.00 0.00 H 821 HG LEU A 53 17.336 76.870 13.377 1.00 0.00 H 822 1HD1 LEU A 53 16.830 79.056 13.024 1.00 0.00 H 823 2HD1 LEU A 53 18.521 79.331 13.257 1.00 0.00 H	
45	ATOM ATOM ATOM ATOM ATOM	825 1HD2 LEU A 53 16.302 76.848 11.201 1.00 0.00 H 826 2HD2 LEU A 53 17.862 77.101 10.346 1.00 0.00 H 827 3HD2 LEU A 53 17.544 75.602 11.226 1.00 0.00 H 828 N ASN A 54 18.372 77.405 15.998 1.00 0.09 N	
50	ATOM ATOM ATOM ATOM ATOM	830 C ASN A 54 16.131 77.235 16.666 1.00 0.09 C 831 O ASN A 54 15.849 78.395 16.374 1.00 0.09 C 832 CB ASN A 54 17.800 77.421 18.416 1.00 0.09 C 833 CG ASN A 54 16.982 76.612 19.411 1.00 0.09 C 834 16.982 76.612 19.411 1.00 0.09 C	
55	ATOM ATOM ATOM ATOM ATOM	835 ND2 ASN A 54 16.916 77.099 20.679 1.00 0.09 N 836 H ASN A 54 18.265 78.392 15.833 1.00 0.00 H 837 HA ASN A 54 17.682 75.775 17.052 1.00 0.00 H 838 1HB ASN A 54 17.555 78.493 18.473 1.00 0.00 H 839 2HB ASN A 54 18.867 73.300	
60	ATOM ATOM ATOM ATOM ATOM	840 1HD2 ASN A 54 17.381 77.945 20.949 1.00 0.00 H 841 2HD2 ASN A 54 16.363 76.577 21.336 1.00 0.00 H 842 N ILE A 55 15.213 76.255 16.677 1.00 0.08 N 843 CA ILE A 55 13.854 76.575 16.377 1.00 0.08 C	
65	ATOM ATOM ATOM ATOM ATOM	845 O ILEA 55 13.338 75.121 18.178 1.00 0.08 C 846 CB ILEA 55 13.310 75.856 15.178 1.00 0.08 C 847 CG1 ILEA 55 13.293 74.339 15.424 1.00 0.08 C 848 CG2 ILEA 55 14.135 76.277 13.950 1.00 0.08 C 849 CD1 ILEA 55 12.481 73.570	
70	ATOM ATOM ATOM	850 H ILE A 55 12.481 73.570 14.384 1.00 0.08 C 850 H ILE A 55 15.434 75.327 17.030 1.00 0.00 H 851 HA ILE A 55 13.731 77.661 16.238 1.00 0.00 H 852 HB ILE A 55 12.270 76.207 15.038 1.00 0.00 H	

ATOM 855 HIGZ LIE A 55 ATOM 855 HIGZ LIE A 55 ATOM 855 HIGZ LIE A 55 ATOM 856 HIGZ LIE A 55 ATOM 866 HIGZ LIE A 55 ATOM 867 HIGZ LIE A 55 ATOM 868 HIGZ LIE A 55 ATOM 860 HIGZ LIE A 55 ATOM 861 N VAL A 56 ATOM 861 N VAL A 56 ATOM 862 CA VAL A 56 ATOM 863 C CA VAL A 56 ATOM 863 C CA VAL A 56 ATOM 863 C CA VAL A 56 ATOM 865 C CO VAL A 56 ATOM 866 C CO VAL A 56 ATOM 867 HIGZ LIE A 55 ATOM 868 HIGZ LIE A 55 ATOM 870 HIGZ LIE A 55 ATOM 871 HIGZ VAL A 56 ATOM 872 HIGZ VAL A 56 ATOM 871 HIGZ VAL A 56 ATOM 872 HIGZ VAL A 56 ATOM 873 HIGZ VAL A 56 ATOM 874 HIGZ VAL A 56 ATOM 877 N ASNA 57 ATOM 876 HIGZ VAL A 56 ATOM 877 N ASNA 57 ATOM 887 HIGZ VAL A 56 ATOM 888 HIGZ VAL A 56 ATOM 887 HIGZ VAL A 56 ATOM 888 HIGZ VAL A 56 ATOM 887 HIGZ VAL A 56 ATOM 887 HIGZ VAL A 56 ATOM 887 HIGZ VAL A 56 ATOM 888 HIGZ VAL A 56 ATOM 888 HIGZ VAL A 56 ATOM 889 HIGZ VAL A 56		ATOM ATOM				0 н
ATOM 856 2He2 LIE A 55 14.181 77.375 13.855 1.00 0.00 H		ATOM	f 855 1HG2 ILE A 5			_
ACCORNEGE Section Se	5		856 2HG2 ILE A 5	5 14.181 77.375		
ATCH 850 2001 112	5		857 3HG2 ILE A 5		14.004 1.00 0.0	-
ATOM 860 N VAI A 56 11.989 76.952 17.851 1.00 0.00 H			859 2HD1 TLE A 5		14.547 1.00 0.00	
ATOM 861 N VAL A 56 11.98 76.902 17.85 1.00 0.00 N			860 3HD1 ILE A 5			
ATCM	1.0		861 N VALA 5		17 27	
ATCH 98.5 C VAL A 56 9,803 76.269 18.333 1.00 0.10 0 ATCH 98.5 CB VAL A 56 10.938 77.689 19.914 1.00 0.10 0 ATCH 98.6 CGI VAL A 56 10.938 77.689 19.914 1.00 0.10 0 ATCH 98.6 CGI VAL A 56 12.308 77.689 19.914 1.00 0.10 C ATCH 98.6 B VAL A 56 11.643 77.623 17.244 1.00 0.00 H ATCH 98.6 B VAL A 56 11.643 77.623 17.244 1.00 0.00 H ATCH 98.6 B VAL A 56 11.643 77.623 17.244 1.00 0.00 H ATCH 97.0 B 18 VAL A 56 10.550 78.573 19.374 1.00 0.00 H ATCH 97.1 B VAL A 56 10.550 78.573 19.374 1.00 0.00 H ATCH 97.1 B VAL A 56 10.078 77.797 1.922 1.00 0.00 H ATCH 97.1 B VAL A 56 10.078 77.797 1.922 1.00 0.00 H ATCH 97.1 B VAL A 56 10.078 77.797 1.922 1.00 0.00 H ATCH 97.1 B VAL A 56 10.078 77.797 1.922 1.00 0.00 H ATCH 97.1 B VAL A 56 12.215 78.754 21.355 1.00 0.00 H ATCH 97.1 B VAL A 56 12.215 78.754 21.355 1.00 0.00 H ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.00 H ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.00 H ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.00 H ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.00 H ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.00 H ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.00 H ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.00 H ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.00 H ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.00 H ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.01 C ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.01 C ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.01 C ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.01 C ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.01 C ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.01 C ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.01 C ATCH 97.1 B VAL A 56 12.294 78.553 19.759 1.00 0.01 C ATCH 97.1 B VAL A 56 12.294 78.554 18.547 1.00 0.11 C ATCH 97.1 B VAL A 56 12.294 78.558 19.494 1.00 0.11 C ATCH 97.1 B VAL A 56 12.294 78.558 19.494 1.00 0.11 C ATCH 97.1 B VAL A 56 12.294 78.558 19.494 1.00 0.11 C ATCH 97.1 B VAL A 56 12.294 78.558 19.494 1.00 0.01 C ATCH 97.1 B VAL A 56 12.294 78.558 19.494 1.0	10		0.00	11.128 76.559		
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15 ATOM 866 CGI VAL A 56			0.55			0
ATOM	1 -					
ATOM 868 H WAL A 566 ATOM 870 HB VAL A 566 ATOM 871 HGI VAL A 566 ATOM 871 HGI VAL A 566 ATOM 872 24GI VAL A 566 ATOM 873 HGI VAL A 566 ATOM 873 HGI VAL A 566 ATOM 873 HGI VAL A 566 ATOM 874 HG2 VAL A 566 ATOM 874 HG2 VAL A 566 ATOM 875 24G2 VAL A 566 ATOM 875 24G2 VAL A 566 ATOM 876 SHG2 VAL A 566 ATOM 877 N ASN A 57 ATOM 878 CA ASN A 57 ATOM 879 C ASN A 57 ATOM 879 C ASN A 57 ATOM 879 C ASN A 57 ATOM 881 CB ASN A 57 ATOM 881 CB ASN A 57 ATOM 882 CG ASN A 57 ATOM 883 ODI ASN A 57 ATOM 883 ODI ASN A 57 ATOM 884 ND2 ASN A 57 ATOM 885 ASN A 57 ATOM 886 ASN A 57 ATOM 886 ASN A 57 ATOM 887 HB ASN A 57 ATOM 888 ND ASN A 57 ATOM 888 ASN A 57 ATOM 889 HB ASN A 57 ATOM 886 ASN A 57 ATOM 887 HB ASN A 57 ATOM 887 HB ASN A 57 ATOM 888 ASN A 57 ATOM 886 ASN A 57 ATOM 887 HB ASN A 57 ATOM 888 ASN A 57 ATOM 887 HB ASN A 57 ATOM 888 ASN A 57 ATOM 886 ASN A 57 ATOM 887 HB ASN A 57 ATOM 888 ASN A 57 ATOM 887 HB ASN A 57 ATOM 888 ASN A 57 ATOM 887 HB ASN A 57 ATOM 888 ASN A 57 ATOM 889 HB ASN A 58 ATOM 890 AND ASN A 58 ATOM 890	15		867 CG2 VAL A 56			
20 ATOM 871 IHG1 VAL A 56 10.550 78.573 19.322 1.00 0.00 H ATOM 871 IHG1 VAL A 56 10.550 78.573 19.374 1.00 0.00 H ATOM 873 3HG1 VAL A 56 8.900 77.797 21.322 1.00 0.00 H ATOM 874 IHG2 VAL A 56 8.900 77.663 20.639 1.00 0.00 H ATOM 875 2HG2 VAL A 56 12.215 76.240 21.212 1.00 0.00 H ATOM 876 3HG2 VAL A 56 12.215 78.754 21.355 1.00 0.00 H ATOM 876 3HG2 VAL A 56 12.947 77.183 20.866 1.00 0.00 H ATOM 878 CA ATOM 877 N ASN A 57 7.00 1.00 1.00 H ATOM 878 CA ASN A 57 7.708 75.604 18.579 1.00 0.00 H ATOM 880 0 ASN A 57 7.708 75.604 18.547 1.00 0.11 C ATOM 880 0 ASN A 57 7.234 75.209 16.227 1.00 0.11 C ATOM 881 CB ASN A 57 7.234 75.209 16.227 1.00 0.11 C ATOM 882 CG ASN A 57 7.234 75.509 14.663 17.634 1.00 0.11 C ATOM 883 MAS ASN A 57 7.598 19.303 1.00 0.11 C ATOM 885 HA ASN A 57 7.598 19.303 1.00 0.11 C ATOM 886 HA ASN A 57 7.598 19.303 1.00 0.11 C ATOM 887 HB ASN A 57 7.598 19.303 1.00 0.00 H ATOM 888 2HB ASN A 57 6.662 76.960 19.613 1.00 0.00 H ATOM 889 1HB ASN A 57 6.677 76.960 19.633 1.00 0.00 H ATOM 889 1HB ASN A 57 6.690 19.613 1.00 0.00 H ATOM 889 1HB ASN A 57 7.598 19.303 1.00 0.01 C ATOM 889 1HB ASN A 57 6.690 19.613 1.00 0.00 H ATOM 889 1HB ASN A 57 6.690 19.613 1.00 0.00 H ATOM 889 1HB ASN A 57 7.598 19.303 1.00 0.01 C ATOM 889 1HB ASN A 57 7.598 19.803 1.00 0.00 H ATOM 889 2HB ALA A 58 8.722 73.047 15.556 1.00 0.21 C ATOM 899 0 ALA A 58 8.722 73.047 15.556 1.00 0.21 C ATOM 899 1 N ALA A 58 8.722 73.047 15.556 1.00 0.21 C ATOM 899 1 N ALA A 58 9.157 73.133 17.613 1.00 0.00 H ATOM 899 1 N ALA A 58 9.157 73.133 17.613 1.00 0.00 H ATOM 899 1 N ALA A 58 9.157 73.133 17.613 1.00 0.00 H ATOM 899 1 N ALA A 58 9.157 73.133 17.613 1.00 0.00 H ATOM 899 1 N ALA A 58 9.157 73.133 17.613 1.00 0.00 H ATOM 990 1 N ALA A 58 9.158 73.899 15.00 0.013 1 C ATOM 990 1 N ALA A 58 9.158 73.899 15.00 0.013 1 C ATOM 990 1 N ALA A 58 9.159 73.133 17.613 1.00 0.00 H ATOM 990 1 N ALA A 58 9.159 73.133 17.613 1.00 0.00 H ATOM 990 1 N ALA A 58 9.159 73.133 17.613 1.00 0.00 H ATOM 990 1 N ALA A 58 9.159 73.133 17.613 1.00 0.00 H ATOM 990 1			0.00	11.643 77.623		
20 ATOM 871 HG1 VAL A 56			000		19.322 1.00 0.00	
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ATOM 915 2HG LYS A 59 5.784 75.617 13.863 1.00 0.00 H ATOM 916 1HD LYS A 59 4.154 74.242 15.231 1.00 0.00 H ATOM 917 2HD LYS A 59 2.851 74.742 14.138 1.00 0.00 H ATOM 918 1HE LYS A 59 3.202 77.149 14.846 1.00 0.00 H ATOM 919 2HE LYS A 59 4.527 76.641 15.925 1.00 0.00 H ATOM 920 1HZ LYS A 59 2.435 76.829 17.091 1.00 0.00 H ATOM 921 2HZ LYS A 59 1.719 75.717 16.136 1.00 0.00 H ATOM 922 3HZ LYS A 59 2.937 75.299 17.120 1.00 0.00 H ATOM 923 N PHE A 60 4.477 75.299 17.120 1.00 0.00 H					1.995 1.00 0.00	
ATOM 916 1HD LYS A 59 4.154 74.242 15.231 1.00 0.00 H ATOM 917 2HD LYS A 59 2.851 74.742 14.138 1.00 0.00 H ATOM 918 1HE LYS A 59 3.202 77.149 14.846 1.00 0.00 H ATOM 919 2HE LYS A 59 4.527 76.641 15.925 1.00 0.00 H ATOM 920 1HZ LYS A 59 2.435 76.829 17.091 1.00 0.00 H ATOM 921 2HZ LYS A 59 1.719 75.717 16.136 1.00 0.00 H ATOM 922 3HZ LYS A 59 2.937 75.299 17.120 1.00 0.00 H ATOM 923 N PHE A 60 4.477 71.214 11.20 1.00 0.00 H				F 704		H
ATOM 918 1HE LYS A 59 2.851 74.742 14.138 1.00 0.00 H ATOM 918 1HE LYS A 59 3.202 77.149 14.846 1.00 0.00 H ATOM 920 1HZ LYS A 59 4.527 76.641 15.925 1.00 0.00 H ATOM 921 2HZ LYS A 59 2.435 76.829 17.091 1.00 0.00 H ATOM 921 2HZ LYS A 59 1.719 75.717 16.136 1.00 0.00 H ATOM 922 3HZ LYS A 59 2.973 75.299 17.120 1.00 0.00 H ATOM 923 N PHE A 60 4.477 71.314 11.20 1.00 0.00 H	65		916 1HD LYS A 59			
ATOM 918 1HE LYS A 59 3.202 77.149 14.846 1.00 0.00 H ATOM 919 2HE LYS A 59 4.527 76.641 15.925 1.00 0.00 H ATOM 920 1HZ LYS A 59 2.435 76.829 17.091 1.00 0.00 H ATOM 921 2HZ LYS A 59 1.719 75.717 16.136 1.00 0.00 H ATOM 922 3HZ LYS A 59 2.973 75.299 17.120 1.00 0.00 H ATOM 923 N PHE A 60 4.477 75.299 17.120 1.00 0.00 H	CO		917 2HD LYS A 59			
ATOM 920 1HZ LYS A 59 4.527 76.641 15.925 1.00 0.00 H ATOM 921 2HZ LYS A 59 2.435 76.829 17.091 1.00 0.00 H ATOM 921 2HZ LYS A 59 1.719 75.717 16.136 1.00 0.00 H ATOM 922 3HZ LYS A 59 2.973 75.299 17.120 1.00 0.00 H ATOM 923 N PHE A 60 4.477 71.314 11.20 1.00 0.00 H				3.202 77.149 1	4.846 1.00 0.00	
70 ATOM 921 2HZ LYS A 59 1.719 75.717 16.136 1.00 0.00 H ATOM 922 3HZ LYS A 59 2.973 75.299 17.120 1.00 0.00 H ATOM 923 N PHE A 60 4.477 71.314 11.220 1.00 0.00 H					5.925 1.00 0.00	
70 ATOM 922 3HZ LYS A 59 2.973 75.299 17.120 1.00 0.00 H ATOM 923 N PHE A 60 4.477 71.314 11.200 1.00 0.00 H	7.0					
ATOM 923 N PHE A 60 4 477 71 214 11 222	70		922 3HZ LYS A 59			
		MOTA				

5	IOTA IOTA IOTA IOTA IOTA IOTA IOTA	M 925 C PH M 926 O PH M 927 CB PH M 928 CG PH M 929 CD1 PH	E A 60 E A 60 E A 60 E A 60 E A 60 E A 60	5.09 5.70 2.85 2.87 2.96	70.579 4 69.726 70.016 3 69.034 1 67.682	9.839 9.197 10.632 9.510 9.748	1.00 0.23 1.00 0.23 1.00 0.23 1.00 0.23 1.00 0.23 1.00 0.23	0 0 0
10	ATOM ATOM ATOM ATOM ATOM	931 CE1 PH 932 CE2 PH 933 CZ PH 934 H PH	E A 60 E A 60 E A 60 E A 60	2.977 2.813 2.902 3.633	66.787 68.584 67.236 71.764	7.409	1.00 0.23 1.00 0.23 1.00 0.23 1.00 0.23 1.00 0.00	0 0
15	ATOM ATOM ATOM ATOM ATOM	936 1HB PHE 937 2HB PHE 938 HD1 PHE 939 HD2 PHE	A 60 A 60 A 60 A 60	4.520 2.378 2.278 3.027 2.735	70.957 69.639	11.406 10.321 11.490 10.769	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	H H H H
20	ATOM ATOM ATOM ATOM	941 HE2 PHE 942 HZ PHE 943 N GLU 944 CA GLU	A 60 A 61 A 61	3.056 2.763 2.922 5.095 5.748	65.721 68.947 66.528 71.879 72.420	8.908 6.138 6.584 9.508	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.15	H H H N
25	MOTA ATOM ATOM ATOM ATOM	945 C GLU 946 O GLU 947 CB GLU 948 CG GLU 949 CD GLU	A 61 A 61 A 61 A 61	7.218 7.889 5.528 5.975 5.349	72.152 71.928 73.936 74.676 76.063	8.459 1 7.454 1 8.259 1 9.522 1	.00 0.15 .00 0.15 .00 0.15 .00 0.15	00000
30	ATOM ATOM ATOM ATOM ATOM	950 OE1 GLU 951 OE2 GLU 952 H GLU 953 HA GLU 954 1HB GLU	A 61 A 61 A 61	5.260 4.938 4.636 5.382 4.456	76.667 76.533 72.552 71.916 74.129	8.408 1 10.605 1 10.097 1 7.445 1	.00 0.15 .00 0.15 .00 0.15 .00 0.00	С 0 01- н н
35	ATOM ATOM ATOM ATOM ATOM	955 2HB GLU 956 1HG GLU 957 2HG GLU 958 N ASP 959 CA ASP	A 61 A 61 A 61 A 62	6.074 7.066 5.569 7.751	74.289 74.750 74.098 72.147	7.366 1 9.599 1 10.323 1 9.694 1	.00 0.00 .00 0.00 .00 0.00 .00 0.00	H H H N
40	ATOM ATOM ATOM ATOM ATOM	960 C ASP 961 O ASP 962 CB ASP 963 CG ASP	A 62 A 62 A 62 A 62	9.160 9.664 10.828 9.539 9.413		9.421 1. 9.041 1. 11.419 1.	00 0.16 00 0.16 00 0.16 00 0.16 00 0.16	00000
45	ATOM ATOM ATOM ATOM	964 OD1 ASP 1 965 OD2 ASP 1 966 H ASP 1 967 HA ASP 1 968 1HB ASP 1	A 62 A 62 A 62	9.712	74.412 1 73.914 1 72.371 1 72.751	10.883 1. 13.000 1. 10.507 1. 9.343 1.	00 0.16 00 0.16 00 0.00 00 0.00	0 01- H H
50	ATOM ATOM ATOM	969 2HB ASP P 970 N SER P 971 CA SER A 972 C SER A	62 63 63 63	9.012 8.832 9.308	71.445 1 69.622 68.342	1.527 1. 2.095 1. 9.415 1. 8.962 1. 7.579 1.	00 0.00 00 0.20 00 0.20	H H N C
	ATOM ATOM ATOM ATOM ATOM	973 O SER A 974 CB SER A 975 OG SER A 976 H SER A 977 HA SER A	63 63 63	9.321 8.213 7.222 7.856	69.189 67.262 67.611 69.781	6.734 1.0 8.921 1.0 7.966 1.0 9.622 1.0	00 0.20 00 0.20 00 0.20 00 0.00	С О Н
55	ATOM ATOM ATOM ATOM ATOM	978 1HB SER A 979 2HB SER A 980 HG SER A 981 N GLY A	63 63 63 64	7.772 6 8.648 6 6.731 6 11.016 6	57.106 9 56.313 8 58.382 8	9.673 1.0 9.916 1.0 3.584 1.0 3.306 1.0 7.328 1.0	0 0.00 0 0.00 0 0.00	H H H N
60	ATOM ATOM ATOM ATOM	982 CA GLY A 983 C GLY A 984 O GLY A 985 H GLY A 986 1HA GLY A	64 1 64 1	13.081 6 13.461 6 11.410 6	7.892 6 7.501 6 6.997 7 7.173 8	5.044 1.0 5.233 1.0 7.288 1.0 7.006 1.0	0 0.22 0 0.22 0 0.22 0 0.00	С С
6 5	ATOM ATOM ATOM ATOM	987 2HA GLY A 988 N GLU A 989 CA GLU A 990 C GLU A	64 1 65 1 65 1 65 1	1.200 6 3.918 6 5.307 6	7.149 5 7.728 5 7.383 5	.553 1.00 .359 1.00 .199 1.00 .302 1.00 .515 1.00	0.00 0.19 0.19	H H N C
70	ATOM ATOM ATOM ATOM	991 O GLU A 992 CB GLU A 993 CG GLU A 994 CD GLU A	65 1 65 1	5.711 69 5.910 66 5.403 65	9.702 5 6.744 4 5.337 3	.000 1.00 .040 1.00 .730 1.00	0.19 0.19 0.19	C 0 C C

	ATO ATO ATO	M 996 (M 997)	DE1 GLU A DE2 GLU A H GLU A HA GLU A	65	16.40 16.62 13.59 15.41	5 63.63 2 68.11	5 2.58 8 4.32	4 1.00 3 1.00	0.19 0.19 0.00	о 01- н
5	OTA OTA OTA OTA	M 999 11 M 1000 21 M 1001 11 M 1002 21	HB GLU A HB GLU A HG GLU A HG GLU A	65 65 65 65	16.99 15.74 14.33 15.57	6 66.696 3 67.417 4 65.361 6 64.670	5 4.21 7 3.18 1 3.47	1 1.00 2 1.00 3 1.00	0.00 0.00 0.00 0.00	н н н н
10	ATON ATON ATON ATON	1 1004 C 1 1005 C 1 1006 C	A TYR A	66 66 66 66	17.16 17.97 19.34 19.83 18.12	0 69.718 2 69.441 9 68.318	6.30 6.54 6.020 6.099	1.00 1.00 1.00 1.00	0.22 0.22 0.22 0.22	и С О
15	ATOM ATOM ATOM ATOM	1 1009 C 1 1010 C 1 1011 C	G TYR A D1 TYR A D2 TYR A E1 TYR A	66 66 66	16.782 15.918 16.382 14.679	70.448 69.482 71.764 69.825	8.567 9.033	1.00 1.00 1.00	0.22 0.22 0.22 0.22 0.22	00000
20	ATOM MOTA MOTA MOTA	1013 C 1014 OI 1015 H	TYR A	66 66 66 66	15.144 14.291 13.021 17.342 17.532	71.143 71.499 67.720	9.078 9.544 10.044 6.847	1.00 1.00 1.00 1.00	0.22 0.22 0.22 0.00	С С О Н
25	ATOM ATOM ATOM ATOM ATOM	1018 2HH 1019 HI 1020 HI	TYR A TYR A TYR A TYR A TYR A	66 66 66	18.806 18.599 16.191 17.046	70.937 69.314 68.433 72.541	6.047 8.084 8.651 9.006 8.220	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
30	ATOM ATOM ATOM ATOM ATOM	1022 HE 1023 HH 1024 N 1025 CA	LYS A LYS A	66 66 67 67	13.997 14.837 12.339 19.979 21.299	73.158 71.120 70.475 70.333	9.847 9.089 9.464 5.440 4.900		0.00 0.00 0.00 0.45 0.45	H H H N C
35	MOTA ATOM ATOM MOTA	1027 O 1028 CB 1029 CG 1030 CD	LYS A LYS A LYS A LYS A LYS A	67 67 67 67 67	22.038 21.429 21.302 20.591 20.205	71.587 72.627 70.211 68.953 69.019	5.238 5.482 3.371 2.871 1.394	1.00 1.00 1.00 1.00	0.45 0.45 0.45 0.45	с 0 с
40	ATOM ATOM ATOM ATOM ATOM	1031 CE 1032 NZ 1033 H 1034 HA 1035 1HB	LYS A LYS A LYS A	67 67 67 67 67	18.982 17.786 19.577 21.802	69.902 69.303 71.404 69.466	1.129 1.761 5.412 5.361	1.00 (1.00 (1.00 (0.45 0.45 0.45 0.00	C C N1+ H H
45	ATOM ATOM ATOM ATOM	1036 2HB 1037 1HG 1038 2HG 1039 1HD	LYS A LYS A LYS A	67 67 67	22.349 20.856 19.696 21.325 19.999	70.191 71.125 68.714 68.161 68.030	3.016 2.952 3.468 3.088 0.954	1.00 0 1.00 0	0.00	н н н н
50	ATOM ATOM ATOM ATOM ATOM	1040 2HD 1041 1HE 1042 2HE 1043 1HZ	LYS A 6	67 67 57	21.053 18.775 19.096 16.927	69.426 69.982 70.919 69.761	0.812 0.049 1.529 1.486	1.00 0 1.00 0 1.00 0	.00 .00 .00 .00	H H H H
	ATOM ATOM ATOM ATOM	1044 2HZ 1045 3HZ 1046 N 1047 CA 1048 C	LYS A 6 CYS A 6 CYS A 6	57 : 58 : 68 :	17.669 17.829 23.383 24.163 25.428	68.327 69.331 71.512 72.670	1.501 2.772 5.281 5.606	1.00 0 1.00 0 1.00 0 1.00 0	.00 .00 .52 .52	H H N C
55	ATOM ATOM ATOM ATOM	1049 O 1050 CB 1051 SG 1052 H	CYS A 6 CYS A 6 CYS A 6 CYS A 6	8 2 8 2 8 2 8 2	5.970 4.621 5.956	72.644 71.578 72.687 73.885 70.694	4.524 7.065 7.311	1.00 0. 1.00 0. 1.00 0.	52	C C S H
60	ATOM ATOM ATOM ATOM ATOM	1053 HA 1054 1HB 1055 2HB 1056 N 1057 CA	CYS A 66 CYS A 66 CYS A 66 GLN A 69 GLN A 69	8 2 8 2 9 2	3.591 4.992 3.803 5.931	73.579 71.688 72.945 73.832	5.374 7.349 7.724 4.420	1.00 0. 1.00 0. 1.00 0.	00 00 00	H H H N
65	ATOM ATOM ATOM ATOM	1058 C 1059 O 1060 CB 1061 CG	GLN A 69 GLN A 69 GLN A 69 GLN A 69 GLN A 69	2 2 2 2	7.926 7.323 7.150	75.086 76.038 73.939	4.234 1 4.727 1 2.237 1	1.00 0. 1.00 0. 1.00 0.	27 (27 (27 (27 (c c c
70	ATOM ATOM	1062 CD 1063 OE1 1064 NE2	GLN A 69 GLN A 69 GLN A 69 GLN A 69	25	6.687 7 7.435 7 5.967 7	75.210 74.400 - 76.130 -	0.186 1 0.360 1 0.511 1	.00 0. .00 0. .00 0. .00 0.	27 c 27 c 27 h	

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5	OTA OTA OTA OTA	M 1067 1HB GLN A M 1068 2HB GLN A M 1069 1HG GLN A M 1070 2HG GLN A	69 27.798 69 26.598 69 28.189 69 27.185 69 25.497	73.064 73.841 76.031	4.081 1.00 0.00 1.859 1.00 0.00 1.876 1.00 0.00 2.029 1.00 0.00 2.036 1.00 0.00	H H H
10	ATOM ATOM ATOM ATOM	1 1072 2HE2 GLN A 1 1073 N HIS A 1 1074 CA HIS A	69 25.234 69 25.927 70 29.263 70 30.076 70 30.899	76.647 75.922 75.063 76.188	-0.068 1.00 0.00 -1.496 1.00 0.00 4.102 1.00 0.11 4.443 1.00 0.11	H H H N C
15	MOTA MOTA MOTA MOTA MOTA	1 1076 O HIS A 1 1077 CB HIS A 1 1078 CG HIS A 1 1079 ND1 HIS A	70 30.877 70 31.043 70 30.339 70 29.937	76.470 75.716 75.946 75.869 76.975	3.237 1.00 0.11 2.267 1.00 0.11 5.612 1.00 0.11 6.930 1.00 0.11 7.646 1.00 0.11	C C N
20	ATOM ATOM ATOM ATOM ATOM	1081 CE1 HIS A 1082 NE2 HIS A 1083 H HIS A 1084 HA HIS A	70 29.331 70 29.316 70 29.699 70 29.447	74.791 76.515 75.195 74.376 77.067	7.664 1.00 0.11 8.768 1.00 0.11 8.824 1.00 0.11 3.501 1.00 0.00 4.660 1.00 0.00	C N H H
25	ATOM ATOM ATOM ATOM	1086 2HB HIS A 1087 HD2 HIS A 1088 HE1 HIS A 1089 HE2 HIS A	70 31.767 70 31.637 70 30.099 70 29.020 70 29.016	76.777 75.036 73.743 77.159 74.625	5.657 1.00 0.00 5.471 1.00 0.00 7.447 1.00 0.00 9.580 1.00 0.00	H H H
	ATOM ATOM ATOM ATOM ATOM	1091 CA GLN A 7 1092 C GLN A 7 1093 O GLN A 7	71 31.625 71 32.441 71 33.468 71 33.753 71 33.197	77.600 77.912 76.834 76.341 79.243	3.251 1.00 0.12 2.121 1.00 0.12 2.009 1.00 0.12 0.920 1.00 0.12	H C C O
30	MOTA MOTA MOTA MOTA	1095 CG GLN A 7 1096 CD GLN A 7 1097 OE1 GLN A 7 1098 NE2 GLN A 7	1 32.304 1 31.895 1 32.123 1 31.272 1 31.670	80.487 80.783 79.983 -	2.276 1.00 0.12 2.279 1.00 0.12 0.843 1.00 0.12 0.063 1.00 0.12 0.623 1.00 0.12	C C C N
35	ATOM ATOM ATOM ATOM ATOM	1100 HA GLN A 7 1101 1HB GLN A 7 1102 2HB GLN A 7 1103 1HG GLN A 7 1104 2HG GLN A 7	1 31.834 1 33.962 1 33.758 1 32.874	77.889 79.321 79.212 81.347	1.204 1.00 0.00 1.481 1.00 0.00 3.225 1.00 0.00 2.668 1.00 0.00	H H H H H
40	ATOM ATOM ATOM ATOM ATOM	1105 1HE2 GLN A 7; 1106 2HE2 GLN A 7; 1107 N GLN A 7; 1108 CA GLN A 7;	1 31.126 1 31.056 2 34.046 2 35.117	82.615 82.232 - 6 76.440 3 75.489	1.391 1.00 0.00 0.322 1.00 0.00 3.157 1.00 0.21	H H H N C
45	ATOM ATOM ATOM ATOM	1110 O GLN A 72 1111 CB GLN A 72 1112 CG GLN A 72 1113 CD GLN A 72	35.308 35.698 36.104 37.057	73.483 1 75.320 4 76.644 5	2.761 1.00 0.21 (1.940 1.00 0.21 (
50	ATOM ATOM ATOM ATOM ATOM	1114 OE1 GLN A 72 1115 NE2 GLN A 72 1116 H GLN A 72 1117 HA GLN A 72 1118 1HB GLN A 72	37.224 7 33.776 7 35.857 7	76.784 3 78.701 4 76.855 4 75.781 2	3.400 1.00 0.21 0 1.547 1.00 0.21 M 1.029 1.00 0.00 H 1.433 1.00 0.00 H) [[
55	ATOM ATOM ATOM ATOM ATOM	1119 2HB GLN A 72 1120 1HG GLN A 72 1121 2HG GLN A 72 1122 1HE2 GLN A 72	34.952 7 36.614 7 35.212 7 36.792 7	4.810 5 6.581 6 7.270 5 9.141 5	.507 1.00 0.00 H .225 1.00 0.00 H .211 1.00 0.00 H .418 1.00 0.00 H .341 1.00 0.00 H	
60	ATOM ATOM ATOM ATOM	1124 N VAL A 73 1125 CA VAL A 73 1126 C VAL A 73 1127 O VAL A 73	33.516 7: 33.130 7: 32.145 7:	3.660 3. 2.297 3. 2.164 1.	.967 1.00 0.00 H .298 1.00 0.31 N .072 1.00 0.31 C .959 1.00 0.31 C	
65	ATOM ATOM	1128 CB VAL A 73 1129 CG1 VAL A 73 1130 CG2 VAL A 73 1131 H VAL A 73 1132 HA VAL A 73	32.521 73 33.583 71 31.247 72 32.902 74	1.650 4. 1.602 5. 2.424 4. 1.241 3.	.283 1.00 0.31 C .395 1.00 0.31 C .666 1.00 0.31 C .836 1.00 0.00 H	
70	ATOM ATOM	1133 HB VAL A 73 1134 1HG1 VAL A 73 1135 2HG1 VAL A 73 1136 3HG1 VAL A 73	32.166 70 33.219 71 34.505 71).641 4. 046 6. 104 5.	786 1.00 0.00 H 101 1.00 0.00 H 275 1.00 0.00 H 053 1.00 0.00 H 740 1.00 0.00 H	

	ATC	M 1137	HG2 VAL	A 7.	3 31.2	60 72.69	7 5 70		_	
	ATC	M 1138 2	HG2 VAL	A 7		74 73.37			0.00 H	
	ATC	M 1139	HG2 VAL	A 7	3 30.3				0.00 H	
5	ATO		n asn						0.00 H 0.41 N	
J	ATO		CA ASN			32 70.45				
	ATO		C ASN						0.41 C	
	ATO ATO		O ASN						0.41 0	
	ATO		CB ASN				7 0.200		0.41 C	
10	ATO		CG ASN OD1 ASN	A 74					0.41 C	
	ATO		ND2 ASN						0.41 0	
	ATO		H ASN				7 -1.542		0.41 N	
	ATO		HA ASN						0.00 H	
	ATO:								0.00 H	
15	ATO	f 1151 2	HB ASN		32.27				0.00 H	
	ATON	1152 1	HD2 ASN	A 74					0.00 н	
	ATON.	1153 2	HD2 ASN	A 74				1.00	0.00 н	
	ATOM	f 1154 j	V GLU		28.56			1.00	0.00 н	
20	ATOM		CA GLU	A 75	27.24	9 69.863		1.00 1.00	0.48 N	
20	ATOM		GLU		27.24			1.00	0.48 C	
	ATOM		GLU.		27.92			1.00	0.48 C 0.48 O	
	ATOM		B GLU	-	26.17	0 69.500	0.145	1.00	_	
	MOTA		G GLU		26.04	7 70.526	-0.982	1.00	0.48 C 0.48 C	
25	ATOM		D GLU		25.36	7 71.763	-0.418	1.00	0.48 C	
20	ATOM ATOM		E1 GLU	A 75	24.69		0.643	1.00	0.48	
	ATOM		E2 GLU		25.50		-1.039	1.00	0.48 01-	
	ATOM		GLU /		28.65		-0.346		0.00 H	
	ATOM	1165 1H			27.01		1.621		0.00 н	
30	MOTA	1166 2H			25.20		0.665		0.00 н	
	ATOM	1167 1H			26.423		-0.272	1.00	0.00 H	
	ATOM	1168 2H			25.416		-1.797	1.00	0.00 H	
	ATOM	1169 N		-	27.009 26.469		-1.450	1.00	0.00 H	
	ATOM	1170 C			26.382		3.309		0.42 N	
35	ATOM	1171 C	SER A		25.336		4.377		0.42 C	
	MOTA	1172 O			24.507		4.009		0.42 C	
	ATOM	1173 CI			25.956	- · · ·	3.136		0.42 0	
	ATOM	1174 00			25.873		5.710		0.42 C	
4.0	ATOM	1175 н	SER A		26.027		6.720 3.444		0.42 0	
40	ATOM	1176 на		76	27.347		4.497		0.00 н	
	ATOM	1177 1HE		76	24.918	69.048	5.529		0.00 H	
	ATOM	1178 2HE		76	26.368	69.600	6.179			
	ATOM	1179 но		76	25.075	67.185	6.523).00 H	
45	MOTA ATOM	1180 N	GLU A	77	25.365	65.881	4.660		.31 N	
10	ATOM	1181 CA 1182 C		77	24.357	64.903	4.380		.31 C	
	ATOM		GLU A	77	23.106	65.426	4.998		.31 c	
	ATOM	1183 O 1184 CB	GLU A	77	23.138	66.145			.31 0	
	ATOM	1185 CG		77	24.596	63.527	5.023		.31 c	
50	ATOM	1186 CD	GLU A GLU A	77 77	25.878	62.834	4.571		.31 C	
	ATOM		1 GLU A	77	26.987	63.328		1.00 0	.31 C	
	ATOM		2 GLU A	77	26.707 28.123	63.507			.31 0	
	ATOM	1189 н	GLU A	77	26.123	63.535			.31 01-	
	ATOM	1190 HA	GLU A	77	24.351	65.592			.00 н	
55	ATOM	1191 1HB	GLU A	77	23.730	64.725 62.916	3.293	1.00 0.	.00 н	
	ATOM	1192 2HB	GLU A	77	24.496	63.579			.00 н	
	ATOM	1193 1HG	GLU A	77	26.103	63.000			.00 н	
	ATOM	1194 2HG	GLU A	77	25.778	61.745			.00 н	
60	ATOM	1195 N	PRO A	78	22.004	65.094			.00 н	
60	ATOM	1196 CA	PRO A	78	20.764	65.579			29 N	
	ATOM	1197 C	PRO A	78	20.323	64.843			29 C	
	ATOM	1198 0	PRO A	78	20.684	63.679			29 C	
	ATOM	1199 CB	PRO A	78	19.756	65.509		.00 0.		
65	ATOM	1200 CG	PRO A	78	20.627	65.643		.00 0.		
05	ATOM	1201 CD	PRO A		21.979	65.042		.00 0.3		
	ATOM	1202 HA	PRO A		20.930	66.637		.00 0.0		
	ATOM	1203 1HB	PRO A		18.975	66.271		.00 0.0		
	ATOM	1204 2HB	PRO A		19.253	64.526		.00 0.0		
70	ATOM ATOM	1205 1HG	PRO A		20.743	66.647		.00 0.0		
. 0	ATOM	1206 2HG			20.192	65.085	1.679 1.	.00 0.0		
	-11 011	1207 1HD	PRO A	78 :	22.062	63.992		00 0.0	00 н	

5	ATON ATON ATON ATON ATOM ATOM	M 1209 N M 1210 CA M 1211 C M 1212 O M 1213 CB	PRO A 76 VAL A 79	9 19.55 9 18.97 9 17.50 9 17.055 19.362	7 65.529 8 64.935 7 65.106 5 66.173 2 65.618		1.00 0.00 1.00 0.31 1.00 0.31 1.00 0.31 1.00 0.31	N C C
10	MOTA MOTA MOTA MOTA MOTA	1215 CG2 1216 H 1217 HA 1218 HB 1219 1HG1	VAL A 79 VAL A 79 VAL A 79 VAL A 79 VAL A 79	18.732 19.361 19.257 20.462	64.848 66.506 63.869 65.577	10.638 6.860 8.216 9.567	1.00 0.31 1.00 0.31 1.00 0.00 1.00 0.00	C H H H
15	ATOM ATOM ATOM ATOM ATOM	1220 2HG1 1221 3HG1 1222 1HG2 1223 2HG2 1224 3HG2	VAL A 79 VAL A 79 VAL A 79	19.283	67.547 67.223 65.237 64.939	8.460 9.523 11.607 10.652	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	H H H H
20	ATOM ATOM ATOM ATOM ATOM	1225 N 1226 CA 1227 C 1228 O 1229 CB	TYR A 80 TYR A 80 TYR A 80 TYR A 80 TYR A 80	16.709 15.305 14.649 14.925 14.628	64.061 64.228 64.401	8.294 1 8.067 1 9.394 1 10.343 1	1.00 0.00 1.00 0.19 1.00 0.19 1.00 0.19 1.00 0.19 1.00 0.19	н С С
25	ATOM ATOM ATOM ATOM ATOM ATOM	1232 CD2 1233 CE1 1234 CE2	TYR A 80 TYR A 80 TYR A 80 TYR A 80 TYR A 80	13.244 12.214 12.983 10.942 11.714	63.476 63.344 64.029 63.754 64.441	7.018 1 7.921 1 5.785 1 7.597 1	.00 0.19 .00 0.19 .00 0.19 .00 0.19 .00 0.19	00000
30	MOTA MOTA MOTA MOTA MOTA	1236 OH 1237 H 1238 HA 1239 1HB	TYR A 80	10.692 9.387 17.008 15.134 14.633	64.301 64.723 63.184 65.090 62.141	6.360 1 6.025 1 8.683 1 7.415 1	.00 0.19 .00 0.19 .00 0.00 .00 0.00	С О Н Н
35	ATOM ATOM ATOM ATOM ATOM	1241 HD1 1 1242 HD2 1 1243 HE1 1 1244 HE2 1	TYR A 80 TYR A 80 TYR A 80	15.197 12.423 13.756 10.137 11.519	62.785 62.901 64.049 63.698 64.850	6.450 1. 8.890 1. 5.036 1. 8.310 1.	00 0.00 00 0.00 00 0.00 00 0.00 00 0.00	н н н н
40	ATOM ATOM ATOM ATOM ATOM	1246 N I 1247 CA I 1248 C I 1249 O I	EU A 81 EU A 81 EU A 81 EU A 81	8.972 13.760 13.094 11.635 11.076	65.671 1 65.423 1 65.757	9.490 1. 0.729 1. 0.529 1. 9.485 1.	00 0.00 00 0.08 00 0.08 00 0.08	H C C
45	ATOM ATOM ATOM ATOM ATOM	1251 CG L 1252 CD1 L 1253 CD2 L 1254 H L	EU A 81 EU A 81		67.437 13 66.632 13 68.948 12 65.997 8	1.191 1. 2.522 1. 3.678 1. 2.800 1. 3.697 1.6	00 0.08 00 0.08 00 0.08	с С С
50	ATOM ATOM ATOM ATOM ATOM	1256 1HB LI 1257 2HB LI	EU A 81 EU A 81 EU A 81 EU A 81	12.768 14.319 11.483 12.405	67.742 10 67.393 11 67.141 12	1.494 1.0 1.414 1.0 1.257 1.0 1.421 1.0 1.427 1.0	0.00 0.00 0.00 0.00	н н н н
55	ATOM ATOM ATOM	1261 3HD1 LE 1262 1HD2 LE 1263 2HD2 LE 1264 3HD2 LE	U A 81 U A 81 U A 81 U A 81	13.915 (11.952 (13.519 (12.001 (65.731 13 67.235 14 69.171 13 69.368 12	.359 1.0 .207 1.0 .726 1.0 .903 1.0 .981 1.0	0.00 0.00 0.00 0.00	H H H H H
60	ATOM ATOM ATOM ATOM	1266 CA GL 1267 C GL 1268 O GL 1269 CB GL	U A 82 U A 82 U A 82 U A 82 U A 82	9.582 6 8.969 6 9.443 6 9.250 6	54.537 11 55.149 12 54.940 13 53.035 11	.529 1.0 .444 1.0 .660 1.0 .776 1.0 .486 1.0	0 0.09 0 0.09 0 0.09 0 0.09	C C C
65	ATOM : ATOM : ATOM :	1271 CD GL1 1272 OE1 GL0 1273 OE2 GL0 1274 H GL0	JA 82 JA 82	9.587 6 8.557 6 10.477 5 11.437 6	2.251 10. 0.767 10. 0.408 11. 9.972 10.	282 1.00 568 1.00 201 1.00 166 1.00 385 1.00	0.09 0.09 0.09 0.09	C C O O1- H
70	ATOM 1	1275 HA GLU 1276 1HB GLU 1277 2HB GLU 1278 1HG GLU	JA 82 JA 82	9.165 6: 8.149 6: 9.643 6:	4.964 10. 2.967 11. 2.600 12.	521 1.00 523 1.00 420 1.00 073 1.00	0.00 0.00 0.00	н н н н

	ATO ATO		HG GLU N VAI		. · · · -				0.00	F
	ATO	M 1281	CA VAL	A 8					0.09	N
5	OTA OTA		VAL			07 65.9	28 13.71	1 1.00	0.09	C
	ATO	1 1284	B VAL						0.09	0
	ATOR ATOR		G1 VAL	A 83	8.4	51 68.6			0.09	C
	ATON		G2 VAL VAL				8 12.25	0 1.00	0.09	c
10	ATON	1288 F	A VAL						0.00	H
	ATON MOTA		B VAL	A 83	6.55	8 68.38	5 14.379		0.00	H H
	ATOM	1290 In	G1 VAL	A 83					0.00	н
15	ATOM	1292 3H	G1 VAL	A 83					0.00	H
10	ATOM ATOM		G2 VAL	A 83		8 69.06	1 11.601	1.00	0.00	H H
	ATOM	1295 Зн	G2 VAL	A 83					0.00	H
	ATOM	1296 N	PHE	A 84					0.00 0.23	H N
20	ATOM ATOM				4.18		4 15.076	1.00	0.23	C
	MOTA	-			3.45 4.07				0.23	С
	ATOM	1300 C			4.22			1.00 1.00	0.23	0
	ATOM ATOM	1301 Co	F PHE		5.21		3 14.810	1.00	0.23	c
25	ATOM		2 PHE		4.88 6.48			1.00	0.23	С
	ATOM ATOM	1304 CI	E1 PHE .	A 84	5.81	4 61.522		1.00 1.00	0.23 0.23	C
	ATOM	1305 CI 1306 CZ	2 PHE		7.414 7.083			1.00	0.23	c
30	ATOM	1307 H	PHE		6.045			1.00 1.00	0.23	C
30	ATOM ATOM	1308 HA 1309 1HE			3.619	65.035	14.132	1.00	0.00	H H
	ATOM	1310 2HB			3.221 4.503				0.00	H
	ATOM	1311 HD	1 PHE 2	84	3.881				0.00 0.00	H
35	ATOM ATOM		2 PHE 2 1 PHE 2		6.776	63.092	16.211		0.00	H H
	ATOM	1314 HE			5.532 8.434				0.00	H
	MOTA	1315 HZ	PHE A	84	7.738	60.588	14.641 13.011		0.00 0.00	H H
	MOTA MOTA	1316 N 1317 CA	SER A		2.115 1.395		16.131	1.00	0.34	N
40	MOTA	1318 C	SER A		0.673	66.292 65.190	17.204 17.915		0.34	C
	ATOM ATOM	1319 O 1320 CB	SER A		-0.388	64.740	17.488		0.34	0
	ATOM	1321 OG	SER A		0.370 -0.610	67.346 66.760	16.748	1.00	34	С
45	MOTA	1322 H	SER A	85	1.591	65.046	15.906 15.547).34).00	О
40	MOTA MOTA	1323 HA 1324 1HB	SER A SER A		2.077	66.796	17.905		.00	H
	ATOM	1325 2HB	SER A	85 85	0.858 -0.105	68.148 67.775	16.180 17.647		.00	H
	ATOM ATOM	1326 HG	SER A	85	-0.897	65.942	16.364		.00	H H
50	ATOM	1327 N 1328 CA	ASP A ASP A	86 86	1.255	64.718	19.032	1.00 0	.23	N
	ATOM	1329 C	ASP A	86	0.646 0.958	63.662 63.925	19.785 21.219		.23	C
	MOTA MOTA	1330 O 1331 CB	ASP A	86	1.850	64.710	21.535	1.00 0 1.00 0	.23 .23	С 0
	MOTA	1331 CB 1332 CG	ASP A	86 86	1.2 0 9 0.750	62.269	19.458	1.00 0	.23	С
55	MOTA	1333 OD1	ASP A	86	-0.436	61.889 62.161	18.058 17.730		.23	С
	ATOM ATOM		ASP A	86	1.581	61.328			.23 .23	0 01-
	ATOM	1335 H 1336 HA	ASP A	86 86	2.097 -0.450	65.076 63.676	19.438	1.00 0.	.00	н
60	ATOM	1337 1HB	ASP A	86	0.728	61.556			.00 .00	H
00	ATOM ATOM	1338 2HB 1339 N	ASP A	86	2.265	62.020	19.445		.00	H H
	ATOM	1339 N 1340 CA	TRP A	87 87	0.199 0.482	63.299			14	N
	ATOM	1341 C	TRP A	87	1.782	63.500 62.871			14	C
65	ATOM ATOM	1342 O 1343 CB	TRP A	87	2.587	63.476				C 0
	ATOM	1344 CG	TRP A	87 87	-0.603 -1.760	62.984			14	С
	ATOM	1345 CD1	TRP A	87	-3.025	63.943 63.873	- ·	.00 0.		C C
	ATOM ATOM		TRP A		-1.660	65.206	25.254 1	.00 0.		C
70	ATOM	1348 CE2	TRP A		-3.722 -2.892			.00 0.	14	N
	ATOM		TRP A		-0.621			.00 0.		C C
							-	•••	'	-

	ATO ATO	M 1351 CZ3 TRP A		67.080 25.67 67.029 26.47		-
_	ATO ATO	1 1000	97 -2.058	67.665 26.35	0 1.00 0.14	С
5	ATO ATO	M 1354 HA TRP A	37 0.614	62.677 21.87 64.581 23.69		
	ATO	1000		62.874 25.48 61.974 24.19	2 1.00 0.00	H
	ATO	M 1357 HD1 TRP A 8	37 -3.478	61.974 24.19 63.070 23.50		H H
10	ATON ATON			55.186 24.20	1.00 0.00	H
	AOTA AOTA	1360 HZ2 TRP A 8	7 -4.070 6	55.286 26.045 57.574 25.578		H H
	ATOM	(1360 mms		7.493 27.066	1.00 0.00	H
15	ATOM ATOM	1 1363 N LEUA 8	8 2.035 6	58.629 26.826 51.637 23.423		H N
	ATOM	1265		0.972 23.818	1.00 0.12	С
	ATOM	1 1366 O LEUA 8	8 3.126 5	0.339 22.607 9.888 21.717		c o
	ATOM ATOM	0		9.838 24.827	1.00 0.12	С
20	ATOM	1369 CD1 LEU A 8		9.089 25.294 9.984 26.135	1.00 0.12 1.00 0.12	C
	ATOM ATOM		8 3.893 5	7.777 26.012	1.00 0.12	C C
	MOTA	1372 HA LEU A 8		1.180 22.722 1.699 24.244	1.00 0.00 1.00 0.00	H
25	ATOM ATOM	1004 000	2.285 59	9.119 24.367	1.00 0.00	H H
	ATOM	1375 HG LEU A 81		0.250 25.711 8.770 24.411	1.00 0.00 1.00 0.00	H
	MOTA MOTA	1077	6.215 59	9.895 25.827	1.00 0.00 1.00 0.00	H H
20	MOTA	1378 3HD1 LEU A 88		1.025 26.171 9.665 27.192	1.00 0.00	H
30	ATOM ATOM	1379 1HD2 LEU A 88 1380 2HD2 LEU A 88	4.792 57	7.191 26.258	1.00 0.00 1.00 0.00	H H
	ATOM	1380 2HD2 LEU A 88		7.971 26.954 7.148 25.391	1.00 0.00	H
	MOTA MOTA	1382 N LEUA 89	5.192 60	.305 22.535	1.00 0.00 1.00 0.11	H N
35	ATOM	1383 C: LEU A 89 1384 C LEU A 89		.659 21.418 .940 21.934	1.00 0.11	С
	MOTA	1385 O LEUA 89	7.608 59	.940 21.934 .330 22.942	1.00 0.11 1.00 0.11	С 0
	ATOM ATOM	1386 CB LEU A 89 1387 CG LEU A 89		.624 20.325	1.00 0.11	С
40	ATOM	1388 CD1 LEU A 89		.930 19.129 .044 18.356	1.00 0.11 1.00 0.11	C C
40	MOTA MOTA	1389 CD2 LEU A 89 1390 H LEU A 89		.949 18.228	1.00 0.11	č
	ATOM	1391 HA LEU A 89		.680 23.262 .108 20.865	1.00 0.00 1.00 0.00	H H
	ATOM ATOM	1392 1HB LEU A 89 1393 2HB LEU A 89		.361 20.757	1.00 0.00	H
45	ATOM	1394 HG LEU A 89		.173 19.917 .325 19.477	1.00 0.00 1.00 0.00	H H
	ATOM ATOM	1395 1HD1 LEU A 89 1396 2HD1 LEU A 89		614 17.450	1.00 0.00	н
	ATOM	1397 3HD1 LEU A 89		.199 18.955 .633 18.029	1.00 0.00 1.00 0.00	H H
50	ATOM ATOM	1398 1HD2 LEU A 89 1399 2HD2 LEU A 89		354 17.418	1.00 0.00	H
	ATOM	1400 3HD2 LEU A 89		683 17.815 485 18.761	1.00 0.00 1.00 0.00	H H
	ATOM ATOM	1401 N LEUA 90 1402 CA LEUA 90	7.400 57.	840 21.259	1.00 0.11	N N
55	ATOM	1403 C LEU A 90	9.606 57.	166 21.649 680 20.677	1.00 0.11 1.00 0.11	C C
33	ATOM ATOM	1404 O LEUA 90 1405 CB LEUA 90	9.404 57.	600 19.467	1.00 0.11	o
	ATOM	1406 CG LEU A 90	9.527 55.6 9.818 54.9		1.00 0.11 1.00 0.11	C
	ATOM ATOM	1407 CD1 LEU A 90 1408 CD2 LEU A 90	10.083 55.	137 23.448	1.00 0.11	C C
60	ATOM	1408 CD2 LEU A 90 1409 H LEU A 90	9.793 53.4 7.168 57.7	704 00	1.00 0.11	С
	MOTA MOTA	1410 HA LEU A 90 1411 1HB LEU A 90	8.845 57.4		1.00 0.00 1.00 0.00	H H
	MOTA	1411 1HB LEU A 90 1412 2HB LEU A 90	8.288 55.3 7.684 55.2	373 20.463	1.00 0.00	H
65	ATOM ATOM	1413 HG LEU A 90	10.652 55.3		1.00 0.00 1.00 0.00	H H
	ATOM	1414 1HD1 LEU A 90 1415 2HD1 LEU A 90	11.099 55.5 9.407 55.8	09 23.615 1	1.00 0.00	H
	MOTA	1416 3HD1 LEU A 90	9.407 55.8 9.922 54.2		.00 0.00	H H
	MOTA MOTA	1417 1HD2 LEU A 90 1418 2HD2 LEU A 90	10.779 52.9	72 21.676 1	.00 0.00	H
70	ATOM	1419 3HD2 LEU A 90	9.069 52.8 9.493 53.3	11 11 1		H
	ATOM	1420 N GLN A 91	10.719 58.2	^^		H N

	ATO OTA	M 1422 M 1423	CA GLNA C GLNA O GLNA	91	11.64 12.85 13.27	57 58.01	8 20.152	1.00	0.11 c
5	ATO ATO ATO ATO	M 1425 (4 1426 (4 1427 (CB GLN A CG GLN A CD GLN A CE1 GLN A	91 91 91	12.09 10.95 11.53 12.41	96 60.25 56 61.27 31 62.58 10 62.58	20.782 3 20.886 2 21.415	1.00 1.00 1.00	0.11 c 0.11 c 0.11 c 0.11 c
10	ATOM ATOM ATOM	1 1429 F 1 1430 F 1 1431 1F	IA GLNA IB GLNA	91 91 91	11.02 10.88 11.16 12.81	6 63.73 0 58.34 4 59.02 6 60.62	0 20.890 1 22.182 9 19.308 9 20.042		0.11 N 0.00 H 0.00 H
15	ATOM ATOM ATOM ATOM ATOM	1433 1H 1434 2H 1435 1H 1436 2H	IG GLN A IG GLN A IE2 GLN A IE2 GLN A	91 91 91 91 91	12.61 10.18 10.46 10.46	4 60.14 4 60.95 4 61.39 9 63.66	7 21.748 1 21.607 1 19.910 0 20.055	1.00 1.00 1.00 1.00	0.00 H 0.00 H 0.00 H 0.00 H
20	MOTA MOTA ATOM ATOM ATOM ATOM	1438 C 1439 C	A ALA A ALA A ALA A	92 92 92 92 92	13.435 14.636 15.533 15.082 14.397	5 58.013 0 57.263 58.108 2 58.925	18.936 18.701 17.870 17.072	1.00 1.00 1.00 1.00	0.18 N 0.18 C 0.18 C 0.18 O
25	ATOM ATOM ATOM ATOM ATOM	1442 H 1443 H 1444 1H 1445 2H 1446 3H	ALA A A ALA A B ALA A B ALA A	92 92 92 92	13.116 15.098 15.351 13.693	58.559 56.977 55.416 55.304	18.152 19.650 17.814 18.463	1.00 1.00 1.00 1.00	0.18 C 0.00 H 0.00 H 0.00 H
30	ATOM ATOM ATOM ATOM	1447 N 1448 C 1449 C 1450 O	SER A	92 93 93 93 93	13.990 16.852 17.796 17.756 17.703	57.959 58.710 58.227		1.00 1.00 1.00 1.00	0.00 H 0.25 N 0.25 C
35	MOTA MOTA MOTA MOTA	1451 CE 1452 OG 1453 H 1454 HA	SER A SER A SER A	93 93 93	19.230 20.123 17.208 17.535	58.542	17.826 17.034 18.779 17.322	1.00 1.00 1.00	0.25 O 0.25 C 0.25 O 0.00 H
	ATOM ATOM ATOM ATOM	1455 1HB 1456 2HB 1457 HG 1458 N 1459 CA	SER A SER A ALA A	93 93 93 94	19.526 19.278 21.022 17.769	57.478 58.881 59.117 56.893	17.807 18.878 17.333 15.694	1.00 (1.00 (1.00 (0.00 H 0.00 H 0.00 H 0.00 H
40	ATOM ATOM ATOM ATOM	1460 C 1461 O 1462 CB 1463 H	ALA A ALA A ALA A	94	17.777 16.919 16.764 19.179	56.384 55.161 54.435 55.986	14.351 14.290 15.271 13.860	1.00 0 1.00 0 1.00 0	0.19 C 0.19 C 0.19 O 0.19 C
45	ATOM ATOM ATOM ATOM	1464 HA 1465 1HB 1466 2HB 1467 3HB	ALA A S ALA A S	94 94 94	17.675 17.357 19.119 19.858	56.216 57.141 55.626 56.852	16.429 13.668 12.821	1.00 0 1.00 0 1.00 0	.00 H .00 H .00 H
50	ATOM ATOM ATOM ATOM	1468 N 1469 CA 1470 C 1471 O	GLU A 9 GLU A 9 GLU A 9	95 95 95	19.610 16.301 15.454 16.282 15.920	55.186 54.943 53.816 52.569 51.545	14.481 13.114 12.861 12.802	1.00 0 1.00 0 1.00 0	.00 H .12 N .12 C
55	ATOM ATOM ATOM ATOM ATOM ATOM	1476 OE2	GLU A 9 GLU A 9 GLU A 9)5 1 5 1 5 1 5 1 5 1	14.711 13.753 13.312 .3.538	53.966 55.164 55.426 54.538 56.522	11.522 1 11.506 1 10.073 1 9.208 1 9.826 1	00 0. 00 0. 00 0.	12 0 12 C 12 C 12 C 12 C 12 O 12 O1-
60	ATOM ATOM ATOM ATOM	1477 H 1478 HA 1479 1HB 1480 2HB 1481 1HG 1482 2HG	GLU A 9 GLU A 9 GLU A 9 GLU A 9 GLU A 9	5 1 5 1 5 1 5 1	4.200	53.702 53.030 54.046 56.089	12.375 1 13.677 1 11.359 1 10.704 1 11.906 1	.00 0.	00 H 00 H 00 H
65	ATOM ATOM ATOM ATOM	1483 N 1484 CA 1485 C	GLU A 95 VAL A 96 VAL A 96 VAL A 96 VAL A 96	6 1 6 1 5 1	7.436 8.234 9.504	54.967 52.630 51.449 51.637	12.134 1 12.110 1 11.956 1 12.709 1	.00 0. .00 0. .00 0.	00 H 11 N 11 C
70	ATOM ATOM ATOM	1487 CB 1488 CG1 1489 CG2 1490 H	VAL A 96 VAL A 96 VAL A 96 VAL A 96 VAL A 96	5 18 5 19 5 17	3.599 9.514 7.299 7.805	51.162 49.924 51.002 53.489	10.531 1. 10.495 1. 9.726 1. 11.747 1.	.00 0.1 .00 0.1 .00 0.1 .00 0.0 .00 0.0	11 C 11 C 11 C

5	ATON ATON ATON ATON ATON ATON ATON	1493 1H 1494 2H 1495 3H 1496 1H 1497 2H 1498 3H	G1 VAL A G1 VAL A G1 VAL A G2 VAL A G2 VAL A G2 VAL A G3	96 19.16 96 19.610 96 20.517 96 19.099 96 17.499 96 16.617 96 16.754	49.588 7 50.203 9 49.089 1 50.648 7 50.282	10.104 9.448 10.851 11.077 8.699 10.198 9.632	1.00 0.0 1.00 0.0 1.00 0.0 1.00 0.0 1.00 0.0	00 H 00 H 00 H 00 H
10	ATOM ATOM ATOM ATOM ATOM ATOM	1500 C 1501 C 1502 O 1503 CE	VALA 9 VALA 9 VALA 9 VALA 9 VALA 9	27 20.028 27 21.230 27 22.100 27 21.654 7 20.992	50.531 50.600 49.467 48.534 50.432	13.268 14.039 13.620 12.957 15.511	1.00 0.0 1.00 0.1 1.00 0.1 1.00 0.1 1.00 0.1	0 N 0 C 0 C
15	ATOM ATOM ATOM ATOM ATOM	1505 CG 1506 H	VAL A 9 VAL A 9 VAL A 9 VAL A 9	7 19.530 7 21.758 7 21.926	49.050 49.654 51.533 50.382	16.004 15.752 13.277 13.789 16.060	1.00 0.10 1.00 0.10 1.00 0.00 1.00 0.00	0 с 0 н
20	ATOM ATOM ATOM ATOM ATOM	1510 2HG 1511 3HG 1512 1HG 1513 2HG	1 VAL A 9' 1 VAL A 9' 2 VAL A 9' 2 VAL A 9'	7 20.458 7 19.080 7 20.214 7 19.366	51.663 52.583 51.481 48.890 48.957	17.104 15.626 15.680 16.835 15.298	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00) H) H) H
25	ATOM ATOM ATOM ATOM ATOM	1514 3HG 1515 N 1516 CA 1517 C 1518 O 1519 CB	MET A 98 MET A 98 MET A 98 MET A 98	23.386 24.315 24.355 24.093	48.221 49.536 48.497 47.640 48.117	15.413 14.004 13.688 14.909 16.012	1.00 0.00 1.00 0.12 1.00 0.12 1.00 0.12 1.00 0.12	H N C
30	ATOM ATOM ATOM ATOM ATOM	1520 CG 1521 SD 1522 CE 1523 H	MET A 98 MET A 98 MET A 98 MET A 98	25.810 25.466 27.170 23.734	49.029 50.033 49.342 48.804 50.300	13.442 12.286 10.639 10.325 14.559	1.00 0.12 1.00 0.12 1.00 0.12 1.00 0.12 1.00 0.00	C C S C H
35	ATOM ATOM ATOM ATOM	1524 HA 1525 1HB 1526 2HB 1527 1HG 1528 2HG	MET A 98 MET A 98 MET A 98 MET A 98 MET A 98	24.011 26.406 26.107 26.805 25.093	50.510	13.257 14.356 12.241	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	н н н н
40	ATOM ATOM ATOM ATOM ATOM	1529 1HE 1530 2HE 1531 3HE 1532 N 1533 CA	MET A 98 MET A 98 GLU A 99 GLU A 99	27.192 27.854 27.497 24.653 24.662	48.311 49.665 48.081 46.339	9.342 10.300 11.086 14.755	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.10	H H H N
45	ATOM ATOM ATOM ATOM ATOM	1534 C 1535 O 1536 CB 1537 CG 1538 CD	GLU A 99 GLU A 99 GLU A 99 GLU A 99	25.806 26.866 24.838 24.757 24.956	45.976 46.341 44.022 43.196	16.779 1 16.272 1 15.682 1 16.970 1	1.00 0.10 1.00 0.10 1.00 0.10 1.00 0.10	00000
50	ATOM ATOM ATOM ATOM ATOM	1539 OE1 1540 OE2 1541 H 1542 HA 1543 1HB	GLU A 99 GLU A 99 GLU A 99 GLU A 99 GLU A 99	24.323 25.752 24.979 23.696	41.247 1 41.063 1 45.929 1 45.668 1	5.652 1 7.347 1 3.900 1 6.459 1	.00 0.10 .00 0.10 .00 0.00 .00 0.00	С О О1- Н Н
55	ATOM ATOM ATOM ATOM ATOM	1544 2HB 1545 1HG 1546 2HG 1547 N 1548 CA	GLU A 99 GLU A 99 GLU A 99 GLY A 100 GLY A 100	23.975 23.715 25.443 25.599	43.700 1 43.288 1 43.481 1 45.973 1	5.117 1 7.265 1 7.776 1 8.108 1	.00 0.00 .00 0.00 .00 0.00 .00 0.00 .00 0.20 .00 0.20	H H N
60		1550 O 1551 H 1552 1HA 1553 2HA	GLY A 100 GLY A 100 GLY A 100 GLY A 100 GLY A 100	26.474 4 27.034 4 24.793 4 27.635 4	47.770 1: 48.210 2: 45.476 1: 46.198 1:	9.396 1. 0.399 1. 3.493 1. 3.562 1.	.00 0.20 .00 0.20 .00 0.00 .00 0.00	о н с
65	ATOM ATOM ATOM ATOM	1555 CA (1556 C (1557 O (1558 CB (GLN A 101 GLN A 101 GLN A 101 GLN A 101 GLN A 101	25.696 4 25.580 4 24.520 5 23.614 4 25.311 5	8.551 18 9.916 19 0.006 20 9.177 20	3.624 1. 9.038 1. 9.078 1. 9.161 1.	00 0.50 00 0.50 00 0.50 00 0.50 00 0.50	н С С
70	ATOM ATOM	1560 CD G 1561 OE1 G	ELN A 101 ELN A 101 ELN A 101 ELN A 101	23.985 5 23.925 5 22.862 5	0.816 17 2.009 16 2.418 15		00 0.50 00 0.50 00 0.50	С С О И

_	ATOM ATOM ATOM ATOM	1 1564 HA GLN A 10 1 1565 1HB GLN A 10	01 26.589 50.219 19.360 1.00 0.00 01 26.170 50.832 17.236 1.00 0.00) н
5	MOTA MOTA ATOM ATOM ATOM	1567 1HG GLN A 10 1568 2HG GLN A 10 1569 1HE2 GLN A 10 1570 2HE2 GLN A 10	11 23.127 50.886 17.861 1.00 0.00 12 23.855 50.016 16.515 1.00 0.00 13 25.979 52.314 16.347 1.00 0.00 14 25.070 53.427 15.358 1.00 0.00	H H H
10	ATOM ATOM ATOM ATOM	1572 CA PRO A 10 1573 C PRO A 10 1574 O PRO A 10 1575 CB PRO A 10	2 23.702 51.170 21.956 1.00 0.57 2 22.464 51.776 21.956 1.00 0.57 2 22.552 52.542 20.440 1.00 0.57 2 24.375 52.030 23.023 1.00 0.57	N C C O
15	ATOM ATOM ATOM ATOM ATOM	1576 CG PRO A 10 1577 CD PRO A 10 1578 HA PRO A 10 1579 1HB PRO A 10 1580 2HB PRO A 10	2 25.870 51.719 22.846 1.00 0.57 2 26.007 51.366 21.355 1.00 0.57 2 23.501 50.183 22.400 1.00 0.00 2 23.985 51.835 24.034 1.00 0.00	C C H H
20	ATOM ATOM ATOM ATOM ATOM	1581 1HG PRO A 102 1582 2HG PRO A 102 1583 1HD PRO A 102 1584 2HD PRO A 102	2 26.136 50.844 23.462 1.00 0.00 2 26.539 52.537 23.155 1.00 0.00 2 26.352 52.231 20.768 1.00 0.00 2 26.737 50.556 21.257 1.00 0.00	н н н н
25	ATOM ATOM ATOM ATOM	1586 CA LEU A 103 1587 C LEU A 103 1588 O LEU A 103 1589 CB LEU A 103	21.299 51.440 21.973 1.00 0.26 20.081 52.025 21.517 1.00 0.26 19.597 52.884 22.628 1.00 0.26 19.568 52.462 23.782 1.00 0.26 18.971 51.003 21 213 1.00 0.26	N C C O C
30	ATOM ATOM ATOM ATOM ATOM	1590 CG LEU A 103 1591 CD1 LEU A 103 1592 CD2 LEU A 103 1593 H LEU A 103 1594 HA LEU A 103	17.661 51.649 20.720 1.00 0.26 17.856 52.350 10.366 1.00	С С Н
35	ATOM ATOM ATOM ATOM ATOM	1595 1HB LEU A 103 1596 2HB LEU A 103 1597 HG LEU A 103 1598 1HD1 LEU A 103 1599 2HD1 LEU A 103	18.745 50.444 22.129 1.00 0.00 19.330 50.271 20.467 1.00 0.00 17.358 52.425 21.447 1.00 0.00 16.913 52.798 19.010 1.00 0.00	н н н н
40	ATOM ATOM ATOM ATOM ATOM	1600 3HD1 LEU A 103 1601 1HD2 LEU A 103 1602 2HD2 LEU A 103 1603 3HD2 LEU A 103 1604 N PHE A 104	18.182 51.630 18.598 1.00 0.00 15.604 51.038 20.237 1.00 0.00 16.779 49.714 20.160 1.00 0.00 16.227 50.355 21.735 1.00 0.00	н н н н
45	ATOM ATOM ATOM ATOM ATOM	1605 CA PHE A 104 1606 C PHE A 104 1607 O PHE A 104 1608 CB PHE A 104	19.234 54.137 22.312 1.00 0.08 18.730 54.987 23.344 1.00 0.08 17.343 55.343 22.936 1.00 0.08 17.099 55.705 21.785 1.00 0.08 19.527 56.291 23.513 1.00 0.08	N C C O C
50	ATOM ATOM ATOM ATOM	1609 CG PHE A 104 1610 CD1 PHE A 104 1611 CD2 PHE A 104 1612 CE1 PHE A 104 1613 CE2 PHE A 104 1614 CZ PHE A 104	18.986 57.015 24.699 1.00 0.08 19.376 56.664 25.972 1.00 0.08 18.097 58.052 24.540 1.00 0.08 18.881 57.333 27.066 1.00 0.08 17.597 58.725 25.630 1.00 0.08	0000
55	ATOM ATOM ATOM ATOM	1615 H PHE A 104 1616 HA PHE A 104 1617 1HB PHE A 104 1618 2HB PHE A 104 1619 HD1 PHE A 104	19.154 54.483 21.371 1.00 0.00 18.727 54.463 24.309 1.00 0.00 19.477 56.897 22.596 1.00 0.00 20.592 56.046 23.663 1.00 0.00	C H H H
60	ATOM :	1620 HD2 PHE A 104 1621 HE1 PHE A 104 1622 HE2 PHE A 104 1623 HZ PHE A 104 1624 N LEU A 105	18.020 58.419 23.527 1.00 0.00 19.224 57.065 28.062 1.00 0.00 16.936 59.563 25.591 1.00 0.00 17.766 59.003 27.735 1.00 0.00	н н н н
65	ATOM 1 ATOM 1 ATOM 1	1625 CA LEU A 105 1626 C LEU A 105 1627 O LEU A 105 1628 CB LEU A 105 1629 CG LEU A 105	15.028 55.541 23.562 1.00 0.10 14.558 56.470 24.624 1.00 0.10 15.108 56.504 25.724 1.00 0.10 14.079 54.330 23.569 1.00 0.10	N C C O C
70	ATOM 1 ATOM 1 ATOM 1	630 CD1 LEU A 105 631 CD2 LEU A 105 632 H LEU A 105 633 HA LEU A 105	14.388 53.284 22.481 1.00 0.10 13.388 52.118 22.534 1.00 0.10 14.485 53.930 21.090 1.00 0.10 16.573 54.928 24.828 1.00 0.00 14.968 56.061 22.597 1.00 0.00	С С Н Н

0.32

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MOTA
                     1634 1HB
                                LEU A 105
                                             13.123 54.780
                                                              23.234
                                                                      1.00
                                                                             0.00
              MOTA
                     1635 2HB
                                LEU A 105
                                             13.791
                                                     53.897
                                                              24.481
              MOTA
                                                                       1.00
                                                                             0.00
                     1636 HG
                                LEU A 105
                                                                                     H
                                             15.382
                                                     52.848
                                                              22.697
                                                                      1.00
                                                                             0.00
             MOTA
                     1637 1HD1 LEU A 105
                                                                                     Н
                                             13.415
                                                     51.501
                                                              21.622
     5
                                                                      1.00
                                                                             0.00
             ATOM
                     1638 2HD1 LEU A 105
                                                                                     H
                                             13.614
                                                     51.452
                                                              23.383
                                                                      1.00
                                                                             0.00
             MOTA
                                                                                     Н
                     1639 3HD1 LEU A 105
                                             12.364
                                                     52.474
                                                              22.682
                                                                      1.00
                                                                             0.00
             ATOM
                     1640 1HD2 LEU A 105
                                                                                     H
                                             14.787
                                                     53.185
                                                              20.341
                                                                      1.00
                                                                             0.00
                     1641 2HD2 LEU A 105
             ATOM
                                                                                     H
                                             13.499
                                                     54.316
                                                             20.781
                                                                      1.00
                                                                             0.00
             MOTA
                     1642 3HD2 LEU A 105
                                                                                     H
                                             15.189
                                                     54.755
                                                             20.996
   10
                                                                      1.00
                                                                             0.00
             ATOM
                     1643
                          N
                               ARG A 106
                                             13.530
                                                     57.274
                                                             24.307
                                                                      1.00
                                                                             0.15
             MOTA
                                                                                     N
                     1644
                               ARG A 106
                           CA
                                            13.059
                                                     58.210
                                                             25.276
                                                                      1.00
                                                                             0.15
             MOTA
                     1645
                                                                                     C
                           С
                               ARG A 106
                                            11.579
                                                     58.303
                                                             25.130
                                                                      1.00
                                                                            0.15
             MOTA
                     1646
                           0
                               ARG A 106
                                            11.049
                                                     58.285
                                                             24.020
                                                                      1.00
                                                                            0.15
             ATOM
                     1647
                                                                                     0
                           CB
                               ARG A 106
                                            13.663
                                                     59.604
   15
                                                             25.034
                                                                      1.00
                                                                            0.15
             ATOM
                                                                                     С
                    1648
                           CG
                               ARG A 106
                                            13.241
                                                     60.704
                                                             26.004
                                                                      1.00
             MOTA
                                                                            0.15
                                                                                     C
                    1649
                           CD
                               ARG A 106
                                            14.061
                                                     61.978
                                                             25.787
                                                                      1.00
                                                                            0.15
             MOTA
                    1650
                           NE
                               ARG A 106
                                            13.541
                                                     63.034
                                                             26.698
             MOTA
                                                                      1.00
                                                                            0.15
                                                                                    N1+
                    1651
                           CZ
                               ARG A 106
                                            12.993
                                                     64.164
                                                             26.169
                                                                      1.00
                                                                            0.15
                          NH1 ARG A 106
             MOTA
                                                                                     C
                    1652
                                            12.935
                                                    64.310
   20
                                                             24.813
                                                                     1.00
                                                                            0.15
             MOTA
                          NH2 ARG A 106
                                                                                    N
                    1653
                                            12.531
                                                    65.148
                                                             26.995
                                                                      1.00
             ATOM
                    1654
                                                                            0.15
                          H
                               ARG A 106
                                            13.091
                                                    57.282
                                                            23.397
             MOTA
                                                                     1.00
                                                                            0.00
                                                                                    Н
                    1655
                          HA
                              ARG A 106
                                            13.331
                                                    57.888
                                                             26.288
                                                                     1.00
                                                                            0.00
            ATOM
                    1656 1HB
                              ARG A 106
                                                                                    Н
                                            13.453
                                                    59.931
                                                            24.002
                                                                     1.00
                                                                            0.00
            MOTA
                    1657 2HB
                              ARG A 106
                                                                                    H
                                            14.740
                                                    59.440
                                                             25.151
  25
                                                                     1.00
            MOTA
                                                                            0.00
                                                                                    Н
                    1658 1HG
                                            13.146
                              ARG A 106
                                                            27.059
                                                    60.420
                                                                     1.00
                                                                            0.00
            ATOM
                                                                                    H
                    1659 2HG
                              ARG A 106
                                            12.200
                                                    60.978
                                                            25.736
                                                                            0.00
                                                                     1.00
            ATOM
                    1660 1HD
                              ARG A 106
                                                                                    H
                                           13.950
                                                    62.234
                                                            24.738
                                                                     1.00
                                                                           0.00
            MOTA
                              ARG A 106
                                                                                    H
                    1661 2HD
                                           15.136
                                                    61.855
                                                            25.994
                                                                     1.00
            ATOM
                                                                           0.00
                    1662
                          HE
                              ARG A 106
                                           13.936
                                                    63.151
                                                            27.606
  30
                                                                     1.00
                                                                           0.00
            ATOM
                                                                                    Н
                   1663 1HH1 ARG A 106
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                                                    63.518
                                                            24.200
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            ATOM
                   1664
                         2HH1 ARG A 106
                                                                                    H
                                           12.383
                                                    65.056
                                                            24.442
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                                                                           0.00
            MOTA
                   1665
                        1HH2 ARG A 106
                                                                                    Н
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                                                    66.008
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            ATOM
                         2HH2 ARG A 106
                                                                                    Н
                   1666
                                           12.481
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                                                            27.979
                                                                     1.00
            MOTA
                                                                           0.00
                                                                                    Н
                   1667
                         N
                              CYS A 107
                                           10.862
  35
                                                   58.384
                                                            26.266
                                                                     1.00
                                                                           0.16
            MOTA
                                                                                   N
                   1668
                          CA
                              CYS A 107
                                            9.446
                                                   58.560
                                                            26.188
                                                                     1.00
            MOTA
                                                                           0.16
                                                                                   С
                   1669
                              CYS A 107
                          С
                                            9.261
                                                   60.020
                                                            26.416
                                                                    1.00
                                                                           0.16
            MOTA
                   1670
                                                                                   C
                         O
                              CYS A 107
                                            9.650
                                                   60.546
57.792
                                                            27.458
                                                                    1.00
                                                                           0.16
            MOTA
                                                                                   0
                   1671
                         CB
                              CYS A 107
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                                                            27.268
                                                                    1.00
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           ATOM
                   1672
                         SG
                              CYS A 107
                                            9.006
                                                   56.009
                                                            27.207
  40
                                                                    1.00
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                                                                                   S
           MOTA
                              CYS A 107
                   1673
                         H
                                           11.264
                                                   58.413
                                                            27.191
                                                                    1.00
                                                                           0.00
           ATOM
                   1674
                                                                                   H
                         HA
                             CYS A 107
                                            9.063
                                                   58.219
                                                            25.214
                                                                    1.00
                                                                           0.00
           ATOM
                   1675 1HB
                             CYS A 107
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                                                   57.974
                                                            27.085
           ATOM
                                                                    1.00
                                                                           0.00
                                                                                   H
                   1676 2HB
                             CYS A 107
                                            8.887
                                                   58.155
                                                           28.282
                                                                    1.00
                                                                           0.00
                                                                                   Н
           ATOM
                   1677
                         N
                             HIS A 108
                                            8.681
                                                   60.725
 45
                                                           25.429
                                                                    1.00
                                                                          0.11
           ATOM
                                                                                   N
                   1678
                         CA
                             HIS A 108
                                           8.593
                                                   62.147
                                                           25.557
                                                                    1.00
           ATOM
                                                                          0.11
                                                                                   С
                   1679
                         С
                             HIS A 108
                                           7.159
                                                   62.550
                                                           25.545
                                                                    1.00
                                                                          0.11
                                                                                   С
           ATOM
                             HIS A 108
HIS A 108
                   1680
                         0
                                           6.360
                                                   62.037
                                                           24.763
                                                                    1.00
                                                                          0.11
           ATOM
                  1681
                                                                                   0
                         CB
                                           9.321
                                                   62.875
                                                           24.412
                                                                    1.00
                                                                          0.11
           ATOM
                  1682
                                                                                   C
                         CG
                             HIS A 108
                                           9.314
                                                  64.372
                                                           24.517
 50
                                                                    1.00
           ATOM
                                                                          0.11
                  1683
                         ND1 HIS A 108
                                           8.352
                                                  65.173
                                                           23.946
                                                                   1.00
                                                                          0.11
           ATOM
                                                                                  N
                  1684
                         CD2 HIS A 108
                                          10.189
                                                  65.217
                                                           25.126
                                                                   1.00
                                                                          0.11
                                                                                  С
           ATOM
                  1685
                        CE1 HIS A 108
                                          8.693
                                                  66.456
                                                           24.231
                                                                   1.00
                                                                          0.11
           ATOM
                                                                                  C
                  1686
                        NE2 HIS A 108
                                           9.799
                                                  66.533
                                                           24.946
                                                                   1.00
                                                                          0.11
                                                                                  N
          ATOM
                  1687
                        Н
                             HIS A 108
                                           8.344
                                                  60.317
 55
                                                           24.563
                                                                   1.00
                                                                          0.00
                                                                                  Н
          MOTA
                  1688
                        HA
                             HIS A 108
                                           9.067
                                                  62.476
                                                           26.494
                                                                   1.00
                                                                          0.00
          MOTA
                                                                                  H
                  1689 1HB
                             HIS A 108
                                           8.903
                                                  62.553
                                                           23.443
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                                                                          0.00
          MOTA
                  1690 2HB
                                                                                  H
                            HIS A 108
                                          10.372
                                                  62.547
                                                           24.407
                                                                   1.00
                                                                          0.00
          ATOM
                                                                                  H
                  1691
                        HD2
                            HIS A 108
                                          10.626
                                                  64.879
                                                           26.029
                                                                   1.00
                                                                         0.00
          ATOM
                  1692
                                                                                  H
                        HE1 HIS A 108
                                          7.908
                                                  67.175
                                                          24.152
60
                                                                   1.00
                                                                         0.00
          ATOM
                                                                                  Н
                  1693
                        HE2 HIS A 108
                                          9.908
                                                  67.286
                                                          25.608
                                                                   1.00
                                                                         0.00
          ATOM
                                                                                  H
                  1694
                        N
                            GLY A 109
                                          6.805
                                                  63.499
                                                          26.433
                                                                   1.00
                                                                         0.09
          ATOM
                                                                                  N
                  1695
                        CA
                            GLY A 109
                                          5.456
                                                  63.967
                                                          26.515
                                                                   1.00
                                                                         0.09
          MOTA
                                                                                  C
                  1696
                            GLY A 109
                        С
                                          5.417
                                                  65.310
                                                          25.871
                                                                   1.00
                                                                         0.09
          ATOM
                 1697
                                                                                  C
                        0
                            GLY A 109
                                                  66.029
                                          6.414
65
                                                          25.839
                                                                   1.00
                                                                         0.09
          ATOM
                                                                                  0
                 1698
                       н
                            GLY A 109
                                          7.478
                                                  64.019
                                                          26.971
                                                                   1.00
                                                                         0.00
          ATOM
                                                                                  H
                 1699 1HA
                            GLY A 109
                                          5.161
                                                  64.080
                                                          27.574
                                                                  1.00
                                                                         0.00
                                                                                 Н
          MOTA
                 1700 2HA
                            GLY A 109
                                          4.765
                                                  63.247
                                                          26.058
                                                                  1.00
                                                                         0.00
          MOTA
                                                                                 H
                 1701
                       N
                            TRP A 110
                                          4.241
                                                 65.682
                                                          25.339
                                                                  1.00
                                                                         0.32
          MOTA
                 1702
                                                                                 N
                       CA
                            TRP A 110
                                          4.097
                                                 66.934
                                                          24.665
70
                                                                  1.00
                                                                         0.32
                                                                                 С
         ATOM
                 1703
                            TRP A 110
                       С
                                          4.162
                                                 68.019
                                                          25.691
                                                                  1.00
                                                                         0.32
                                                                                 C
         MOTA
                 1704 o
                            TRP A 110
                                          3.707
                                                 67.858
                                                          26.822
                                                                  1.00
```

	ATOM ATOM ATOM	1706 CG	TRP A 110	2.53	34 68.31			0.32	c c
5	ATOM ATOM ATOM	1708 CD: 1709 NE	l TRP A 110 2 TRP A 110 1 TRP A 110 2 TRP A 110	1.52 2.58	69.27 3 69.99	0 23.495 7 21.65	1 1.00 5 1.00 7 1.00	0.32 0.32 0.32	C C N
10	ATOM ATOM ATOM	1711 CES 1712 CZS 1713 CZS	3 TRP A 110 2 TRP A 110 3 TRP A 110	0.62 0.72 -0.23	9 71.36	8 24.517 4 22.620	7 1.00 1.00	0.32 0.32 0.32 0.32	0000
10	ATOM ATOM ATOM ATOM	1714 CH2 1715 H 1716 HA 1717 1HB	TRP A 110 TRP A 110	3.50 4.92	3 71.386 1 64.994 2 67.038	23.653 4 25.214 3 23.933	1.00	0.32 0.00 0.00	C H H
15	ATOM ATOM ATOM	1718 2HB 1719 HD1	TRP A 110 TRP A 110 TRP A 110 TRP A 110	1.92 2.76 4.01 3.07	6 66.199 3 68.408	23.167 21.524	1.00 1.00	0.00 0.00 0.00	Н Н Н
20	ATOM ATOM ATOM	1721 HE3 1722 HZ2 1723 HZ3	TRP A 110 TRP A 110 TRP A 110	0.60 0.77 -1.03	4 68.488 1 72.167	25.237 21.889	1.00	0.00 0.00 0.00	H H H
20	MOTA MOTA MOTA	1724 HH2 1725 N 1726 CA 1727 C	TRP A 110 ARG A 111 ARG A 111 ARG A 111	-0.907 4.775 4.933	72.196 69.157 70.280	23.710 25.311 26.189	1.00 1.00 1.00	0.00 0.53 0.53	H N C
25	ATOM ATOM ATOM	1728 O 1729 CB 1730 CG	ARG A 111 ARG A 111 ARG A 111	5.683 5.653 3.620 3.020	70.566		1.00 1.00 1.00 1.00	0.53 0.53 0.53	0 0 0
30	ATOM ATOM ATOM T.TOM	1731 CD 1732 NE 1733 CZ 1734 NH1	ARG A 111 ARG A 111 ARG A 111 ARG A 111	2.053 0.754 -0.186 0.095	72.917 72.237 72.834	26.245 26.508 27.299 27.921	1.00 1.00 1.00	0.53 0.53 0.53	C C N1+ C
	ATOM ATOM ATOM ATOM	1735 NH2 1736 H 1737 HA	ARG A 111 ARG A 111 ARG A 111 ARG A 111	-1.396 5.186 5.583	72.233 69.239 71.018	27.493 24.389 25.683	1.00 1.00 1.00 1.00	0.53 0.53 0.00 0.00	N N H H
35	ATOM ATOM ATOM	1739 2HB 1740 1HG 1741 2HG	ARG A 111 ARG A 111 ARG A 111	3.792 2.899 2.557 3.855	71.524 70.159 71.368 72.472	27.570 26.910 24.791 25.192	1.00 1.00	0.00 0.00 0.00 0.00	H H H H
40	MOTA MOTA ATOM ATOM	1743 2HD . 1744 HE .	ARG A 111 ARG A 111 ARG A 111 ARG A 111	1.871 2.462 0.400	73.778 73.292 71.687	25.580 27.198 25.751	1.00 1.00 1.00	0.00 0.00 0.00	H H H
<i>A</i> E	ATOM ATOM ATOM	1746 2HH1 2 1747 1HH2 2 1748 2HH2 2	ARG A 111 ARG A 111 ARG A 111	0.986 -0.584 -2.095 -1.585	74.448 74.483 72.648 71.323	27.837 28.480 28.070 27.140	1.00 (0.00 0.00 0.00 0.00	H H H
45	ATOM ATOM ATOM ATOM	1750 CA 2 1751 C 2	ASN A 112 ASN A 112 ASN A 112	6.402 7.191 6.360	68.732 68.280 68.240	27.343 28.452 29.693	1.00 0 1.00 0).33).33).33	H C C
50	ATOM ATOM MOTA	1753 CB A 1754 CG A 1755 OD1 A	SN A 112 SN A 112 SN A 112 SN A 112	6.800 8.409 9.405 9.721	68.685 69.178 68.984 67.852	30.754 28.734 27.605 27.241	1.00 0 1.00 0	.33 .33 .33	0 C C
55	ATOM ATOM ATOM ATOM	1756 ND2 A 1757 H A 1758 HA A	SN A 112 SN A 112 SN A 112	9.908 6.362 7.515	70.110 68.142 67.243	27.031 26.519	1.00 0 1.00 0	.33 .33 .00	O H H
	ATOM ATOM		SN A 112 SN A 112 SN A 112 SN A 112	8.936 8.129 9.555 10.399	71.013	28.898 27.290	1.00 0 1.00 0	.00 .00	H H H
60	ATOM ATOM ATOM	1763 N TI 1764 CA TI 1765 C TI	RP A 113 RP A 113 RP A 113	5.133 4.351 4.945	67.695 67.630	29.612 30.808	1.00 0. 1.00 0.	.00 .13 .13	H C C
65	ATOM ATOM ATOM	1767 CB TF 1768 CG TF 1769 CD1 TF	RP A 113 RP A 113 RP A 113 RP A 113	5.619 2.864 2.109 1.666	65.657 67.316 68.431	31.177 1 30.572 1 29.884 1	1.00 0. 1.00 0. 1.00 0.	.13 .13 .13	0 C C
	ATOM :	1770 CD2 TF 1771 NE1 TF 1772 CE2 TF	P A 113 P A 113 P A 113 P A 113	1.737 1.030 1.071	69.663 3 69.717 2 70.435 2	30.524 1 28.395 1 29.574 1	.00 0. .00 0.	13 13 13	C C N C
70	ATOM	1774 CZ2 TR	P A 113 P A 113 P A 113	0.593	71.676 2	9.891 1	.00 0. .00 0.	13 13	C C

5	ATON ATON ATON	M 1777 H TRP A 113 M 1778 HA TRP A 113 M 1779 1HB TRP A 113	4.706 67.47 4.416 68.60 2.398 67.12	4 28.722 2 31.331	1.00 0.13 1.00 0.00 1.00 0.00 1.00 0.00	C H H H
3	ATOM ATOM ATOM ATOM ATOM	1781 HD1 TRP A 113 1782 HE1 TRP A 113 1783 HE3 TRP A 113	1.720 67.74 0.985 70.17 2.453 69.52	6 30.007 6 27.844 7 27.511 4 32.547	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	H H H H
10	ATOM ATOM ATOM ATOM	1785 HZ3 TRP A 113 1786 HH2 TRP A 113 1787 N ASP A 114	-0.140 72.21 1.587 71.75 0.388 73.096 4.712 66.648 5.293 65.702	3 33.118 6 31.480 8 32.988	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.12	H H H N
15	ATOM ATOM ATOM ATOM	1789 C ASP A 114 1790 O ASP A 114 1791 CB ASP A 114 1792 CG ASP A 114	5.293 65.702 4.813 64.344 3.627 64.137 4.874 65.921 5.445 67.250	33.513 7 33.263 1 35.357	1.00 0.12 1.00 0.12 1.00 0.12 1.00 0.12	0000
20	ATOM ATOM ATOM ATOM	1793 OD1 ASP A 114 1794 OD2 ASP A 114 1795 H ASP A 114 1796 HA ASP A 114	6.688 67.432 4.640 68.101 4.235 67.413 6.396 65.763	35.731 36.285 33.434	1.00 0.12 1.00 0.12 1.00 0.12 1.00 0.00 1.00 0.00	С 0 01- н н
25	ATOM ATOM ATOM ATOM ATOM	1797 1HB ASP A 114 1798 2HB ASP A 114 1799 N VAL A 115 1800 CA VAL A 115 1801 C VAL A 115	5.326 65.104 3.782 65.878 5.746 63.378 5.368 62.043	35.943 1 35.482 1 33.447 1 33.098 1	1.00 0.00 1.00 0.00 1.00 0.21 1.00 0.21	H H N C
30	ATOM ATOM ATOM ATOM ATOM	1802 O VAL A 115 1803 CB VAL A 115 1804 CG1 VAL A 115 1805 CG2 VAL A 115 1806 H VAL A 115	5.975 61.133 7.072 61.378 5.880 61.603 5.413 60.158 5.402 62.604	34.611 1 31.759 1 31.508 1 30.694 1	.00 0.21 .00 0.21 .00 0.21 .00 0.21 .00 0.21	0000
35	ATOM ATOM ATOM ATOM	1807 HA VAL A 115 1808 HB VAL A 115 1809 1HG1 VAL A 115 1810 2HG1 VAL A 115	6.699 63.523 4.271 61.948 6.981 61.596 5.622 59.852 5.940 59.432	33.117 1 31.744 1 30.468 1	.00 0.00 .00 0.00 .00 0.00 .00 0.00	н н н н
40	ATOM ATOM ATOM ATOM ATOM	1811 3HG1 VAL A 115 1812 1HG2 VAL A 115 1813 2HG2 VAL A 115 1814 3HG2 VAL A 115 1815 N TYR A 116	4.326 60.047 6.242 63.234 5.022 62.106 4.626 63.295 5.249 60.058	31.656 1. 30.360 1. 29.788 1. 31.037 1.	.00 0.00 .00 0.00 .00 0.00	н н н н
ΛE	ATOM ATOM ATOM ATOM	1816 CA TYR A 116 1817 C TYR A 116 1818 O TYR A 116 1819 CB TYR A 116	5.249 60.058 5.738 59.110 5.192 57.784 4.387 57.702 5.271 59.408	35.407 1. 34.997 1. 34.070 1.	00 0.44 00 0.44 00 0.44 00 0.44 00 0.44	N C C
45	ATOM ATOM ATOM ATOM	1820 CG TYR A 116 1821 CD1 TYR A 116 1822 CD2 TYR A 116 1823 CE1 TYR A 116	3.794 59.519 2.990 58.419 3.215 60.735 1.624 58.535		00 0.44 00 0.44 00 0.44	00000
50	ATOM ATOM ATOM ATOM ATOM	1824 CE2 TYR A 116 1825 CZ TYR A 116 1826 OH TYR A 116 1827 H TYR A 116 1828 HA TYR A 116	1.851 60.859 1.050 59.757 -0.352 59.883 4.338 59.869	36.391 1.6 36.548 1.6 36.451 1.6 34.060 1.6	00 0.44 00 0.44 00 0.44	C C O H
55	ATOM ATOM ATOM ATOM	1828 HA TYR A 116 1829 1HB TYR A 116 1830 2HB TYR A 116 1831 HD1 TYR A 116 1832 HD2 TYR A 116	3.439 57.467	35.343 1.0 37.186 1.0 37.523 1.0 37.135 1.0	0.00 0.00 0.00	н н н
60	ATOM ATOM ATOM ATOM	1833 HE1 TYR A 116 1834 HE2 TYR A 116 1835 HH TYR A 116 1836 N LYS A 117	0.986 57.727 1.421 61.836 -0.572 60.683 5.625 56.712	36.358 1.0 37.108 1.0 36.180 1.0 35.940 1.0 35.689 1.0	0.00 0.00 0.00	H H H N
65	ATOM ATOM ATOM	1837 CA LYS A 117 1838 C LYS A 117 1839 O LYS A 117 1840 CB LYS A 117 1841 CG LYS A 117	5.361 55.152 4.381 54.992 3.732 55.063	35.366 1.0 33.903 1.0 33.177 1.0 35.716 1.0	0 0.45 0 0.45 0 0.45 0 0.45	с с о с
70	ATOM ATOM ATOM	1842 CD LYS A 117 1843 CE LYS A 117 1844 NZ LYS A 117 1845 H LYS A 117 1846 HA LYS A 117	2.021 54.552 3 1.803 54.093 3 1.648 55.268 3 6.471 56.822 3	37.205 1.00 37.540 1.00 38.982 1.00 39.868 1.00 36.234 1.00 35.905 1.00	0 0.45 0 0.45 0 0.45 0 0.45 0 0.00	C C N1+ H

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1 1848 2HB LYS A 11 1 1849 1HG LYS A 11 1 1850 2HG LYS A 11 1 1851 1HD LYS A 11 1 1852 2HD LYS A 11	7 3.072 55.855 35.321 1.00 0.00 H 7 4.032 55.470 37.906 1.00 0.00 H 7 3.730 53.803 37.280 1.00 0.00 H 7 1.662 53.770 36.846 1.00 0.00 H 7 1.404 55.440 37.399 1.00 0.00 H	
10	ATOM ATOM ATOM ATOM ATOM	1854 2HE LYS A 11: 1855 1HZ LYS A 11: 1856 2HZ LYS A 11: 1857 3HZ LYS A 11: 1858 N VAL A 116	7 0.875 53.505 39.082 1.00 0.00 H 7 1.542 55.010 40.843 1.00 0.00 H 7 2.458 55.876 39.832 1.00 0.00 H 9 0.847 55.842 39.642 1.00 0.00 H 9 6.621 55 134 33 433 1.00	
15	MOTA MOTA MOTA MOTA MOTA	1860 C VAL A 118 1861 O VAL A 118 1862 CB VAL A 118 1863 CG1 VAL A 118	6.873 54.949 32.037 1.00 0.21 C 7.212 53.512 31.806 1.00 0.21 C 7.958 52.902 32.569 1.00 0.21 O 8.032 55.762 31.546 1.00 0.21 C 8.313 55.380 30.088 1 00 0.21 C	
20	ATOM ATOM ATOM ATOM ATOM	1864 CG2 VAL A 118 1865 H VAL A 118 1866 HA VAL A 118 1867 HB VAL A 118 1868 1HG1 VAL A 118	7.708 57.251 31.749 1.00 0.21 C 7.436 55.211 34.029 1.00 0.00 H 5.985 55.278 31.488 1.00 0.00 H 8.930 55.521 32.142 1.00 0.00 H 9.125 56.011 32.606	
25	ATOM ATOM ATOM ATOM ATOM	1869 2HG1 VAL A 118 1870 3HG1 VAL A 118 1871 1HG2 VAL A 118 1872 2HG2 VAL A 118 1873 3HG2 VAL A 118	8.627 54.336 29.946 1.00 0.00 H 7.399 55.589 29.526 1.00 0.00 H 8.495 57.906 31.341 1.00 0.00 H 6.771 57.514 31.231 1.00 0.00 H	
30	MOTA MOTA MOTA MOTA MOTA MOTA	1874 N ILE A 119 1875 CA ILE A 119 1876 C ILE A 119 1877 O ILE A 119 1878 CB ILE A 119	6.636 52.922 30.739 1.00 0.09 N 6.937 51.557 30.434 1.00 0.09 C 7.363 51.496 29.005 1.00 0.09 C 6.814 52.188 28.149 1.00 0.09 O	
35	ATOM ATOM ATOM ATOM ATOM	1879 CG1 ILE A 119 1880 CG2 ILE A 119 1881 CD1 ILE A 119 1882 H ILE A 119 1883 HA ILE A 119	5.244 50.662 32.028 1.00 0.09 C 6.202 49.239 30.108 1.00 0.09 C 3.887 49.980 32.199 1.00 0.09 C 6.019 53.432 30.114 1.00 0.00 H	
40	ATOM ATOM ATOM ATOM ATOM	1884 HB ILE A 119 1885 1HG1 ILE A 119 1886 2HG1 ILE A 119 1887 1HG2 ILE A 119 1888 2HG2 ILE A 119	7.753 51.208 31.079 1.00 0.00 H 4.974 50.986 29.918 1.00 0.00 H 5.127 51.696 32.388 1.00 0.00 H 5.962 50.087 32.618 1.00 0.00 H 5.476 48.458 30.381 1.00 0.00 H	
45	MOTA ATOM ATOM MOTA	1889 3HG2 ILE A 119 1890 1HD1 ILE A 119 1891 2HD1 ILE A 119 1892 3HD1 ILE A 119	6.342 49.174 29.021 1.00 0.00 H 7.135 48.928 30.599 1.00 0.00 H 3.583 50.024 33.259 1.00 0.00 H 3.096 50.494 31.635 1.00 0.00 H	
50	ATOM ATOM ATOM ATOM ATOM ATOM	1893 N TYR A 120 1894 CA TYR A 120 1895 C TYR A 120 1896 O TYR A 120 1897 CB TYR A 120	8.383 50.666 28.722 1.00 0.09 N 8.837 50.488 27.377 1.00 0.09 C 8.350 49.159 26.923 1.00 0.09 C 8.418 48.175 27.658 1.00 0.09 C 10.367 50.494 27.212 1.00 0.09	
55	ATOM ATOM ATOM ATOM	1898 CG TYR A 120 1899 CD1 TYR A 120 1900 CD2 TYR A 120 1901 CE1 TYR A 120 1902 CE2 TYR A 120 1903 CZ TYR A 120	10.850 51.903 27.189 1.00 0.09 C 11.051 52.631 28.339 1.00 0.09 C 11.111 52.492 25.973 1.00 0.09 C 11.504 53.929 28.266 1.00 0.09 C 11.563 53.785 25.893 1.00 0.09 C	
60	ATOM ATOM ATOM	1904 OH TYR A 120 1905 H TYR A 120 1906 HA TYR A 120 1907 1HB TYR A 120	11.761 54.505 27.043 1.00 0.09 C 12.226 55.832 26.949 1.00 0.09 O 8.765 50.046 29.425 1.00 0.00 H 8.416 51.282 26.738 1.00 0.00 H 10.609 49.990 26.261 1.00 0.00 H	
65	ATOM 1 ATOM 1 ATOM 1 ATOM 1	1909 HD1 TYR A 120 1910 HD2 TYR A 120 1911 HE1 TYR A 120 1912 HE2 TYR A 120	10.841 49.895 28.003 1.00 0.00 H 10.804 52.180 29.294 1.00 0.00 H 10.959 51.928 25.055 1.00 0.00 H 11.635 54.510 29.175 1.00 0.00 H	
70	ATOM 1 ATOM 1 ATOM 1		11.814 54.215 24.941 1.00 0.00 H 11.980 56.270 27.778 1.00 0.00 H 7.816 49.106 25.689 1.00 0.18 N 7.302 47.867 25.199 1.00 0.18 C 8.013 47.542 23.925 1.00 0.18 C 8.291 48.417 23.108 1.00 0.18 O	

	OTA OTA OTA	4 1919 CG TYR A 121 4 1920 CD1 TYR A 121	5.083 48.2 4.694 47.1	19 26.150 98 26.987	1.00 0.18 1.00 0.18 1.00 0.18	
5	ACTA ACTA ACTA ACTA	1 1922 CE1 TYR A 121 1 1923 CE2 TYR A 121 1 1924 CZ TYR A 121	4.028 47.46 4.134 49.79 3.744 48.76	59 28.160 92 27.679 58 28.506	1.00 0.18 1.00 0.18 1.00 0.18 1.00 0.18	0000
10	ATOM ATOM ATOM	1 1926 H TYR A 121 1 1927 HA TYR A 121 1 1928 1HB TYR A 121 1 1929 2HB TYR A 121	7.631 49.92	20 25.112 07 25.959 63 24.447	1.00 0.18 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	О Н Н
15	ATOM ATOM ATOM ATOM	1931 HD2 TYR A 121 1932 HE1 TYR A 121 1933 HE2 TYR A 121	4.897 46.16 5.098 50.33 3.695 46.65 4.048 50.84	55 26.711 4 25.859 2 28.797 1 27.783	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	H H H H
20	MOTA MOTA MOTA MOTA MOTA	1935 N LYS A 122 1936 CA LYS A 122 1937 C LYS A 122	2.599 49.88 8.347 46.24 9.000 45.72 8.109 44.63 7.986 43.60	9 23.757 7 22.598 0 22.126	1.00 0.00 1.00 0.28 1.00 0.28 1.00 0.28	H N C
25	ATOM ATOM ATOM ATOM	1939 CB LYS A 122 1940 CG LYS A 122 1941 CD LYS A 122 1942 CE LYS A 122	10.349 45.06 11.176 44.62 12.535 44.03 13.183 44.71	2 22.933 3 21.722 0 22.111	1.00 0.28 1.00 0.28 1.00 0.28 1.00 0.28 1.00 0.28	00000
30	MOTA MOTA MOTA MOTA	1943 NZ LYS A 122 1944 H LYS A 122 1945 HA LYS A 122 1946 1HB LYS A 122 1947 2HB LYS A 122	14.483 44.073 8.145 45.56 9.164 46.523 10.242 44.243 10.988 45.833	23.628 7 24.483 8 21.864 0 23.659	1.00 0.28 1.00 0.00 1.00 0.00 1.00 0.00	N1+ H H H
	MOTA MOTA MOTA MOTA	1948 1HG LYS A 122 1949 2HG LYS A 122 1950 1HD LYS A 122 1951 2HD LYS A 122	10.988 45.835 11.311 45.492 10.623 43.882 13.201 44.012 12.369 42.972	2 21.057 2 21.114 2 21.232	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	н н н н
35	ATOM MOTA ATOM ATOM ATOM	1952 1HE LYS A 122 1953 2HE LYS A 122 1954 1HZ LYS A 122 1955 2HZ LYS A 122	12.551 44.547 13.425 45.746 14.925 44.473 14.393 43.081	24.190 23.185 24.445 23.789	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	H H H H
40	ATOM ATOM ATOM ATOM	1956 3HZ LYS A 122 1957 N ASP A 123 1958 CA ASP A 123 1959 C ASP A 123 1960 O ASP A 123	15.133 44.201 7.464 44.826 6.591 43.826 5.595 43.429 5.193 42.269	20.965 20.428 21.470	1.00 0.00 1.00 0.20 1.00 0.20 1.00 0.20	H C C
45	ATOM ATOM ATOM ATOM	1961 CB ASP A 123 1962 CG ASP A 123 1963 OD1 ASP A 123 1964 OD2 ASP A 123	7.339 42.593 8.044 43.045 7.553 44.021 9.081 42.430	19.901 18.631 18.001	1.00 0.20 1.00 0.20 1.00 0.20 1.00 0.20 1.00 0.20	0 C C 0 01-
50	ATOM ATOM ATOM ATOM ATOM	1965 H ASP A 123 1966 HA ASP A 123 1967 1HB ASP A 123 1968 2HB ASP A 123 1969 N GLY A 124	7.666 45.628 5.968 44.289 6.613 41.815 8.032 42.140	20.369 1 19.639 1 19.612 1 20.623 1	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	H H H H
55	ATOM ATOM ATOM ATOM ATOM	1970 CA GLY A 124 1971 C GLY A 124 1972 O GLY A 124 1973 H GLY A 124	5.173 44.404 4.147 44.159 4.739 43.612 4.011 43.266 5.538 45.337	23.266 1 24.523 1 25.454 1	1.00 0.17 1.00 0.17 1.00 0.17 1.00 0.00	N C C O H
60	MOTA MOTA MOTA MOTA	1974 1HA GLY A 124 1975 2HA GLY A 124 1976 N GLU A 125 1977 CA GLU A 125 1978 C GLU A 125	3.420 43.428 3.606 45.080 6.076 43.516 6.638 42.987 7.229 44.137	23.485 1 24.601 1 25.806 1	.00 0.00 .00 0.00 .00 0.24 .00 0.24	H H N C
65	ATOM ATOM ATOM ATOM ATOM	1979 O GLU A 125 1980 CB GLU A 125 1981 CG GLU A 125 1982 CD GLU A 125 1983 OE1 GLU A 125	7.934 44.962 7.747 41.958 8.099 41.137 9.183 40.146	25.980 1 25.550 1 26.785 1 26.392 1	.00 0.24 .00 0.24 .00 0.24 .00 0.24	0 C C
70	ATOM ATOM ATOM ATOM ATOM	1984 OE2 GLU A 125 1985 H GLU A 125 1986 HA GLU A 125 1987 1HB GLU A 125 1988 2HB GLU A 125	10.013 40.500 9.192 39.023 6.662 43.562 5.870 42.467 8.638 42.476 7.408 41.267	26.962 1. 23.773 1. 26.400 1. 25.156 1.	.00 0.24 .00 0.24 .00 0.00 .00 0.00 .00 0.00	0 01- н н н

5	ATON ATON ATON ATON ATON ATON	M 1990 2HG M 1991 N M 1992 CA M 1993 C M 1994 O	GLU A 12: GLU A 12: ALA A 12: ALA A 12: ALA A 12: ALA A 12: ALA A 12:	8.49 6 6.96 7.48 8.92 9.25	94 41.78 67 44.23 83 45.37 23 45.12 67 44.25	39 27.582 37 27.865 77 28.563 89 28.870 50 29.662	2 1.00 5 1.00 8 1.00 1.00 1.00	0.00 0.26 0.26 0.26 0.26	н и с с
10	MOTA MOTA MOTA MOTA MOTA	1 1997 HA 1 1998 1HB 1 1999 2HB 1 2000 3HB	ALA A 126 ALA A 126 ALA A 126 ALA A 126 ALA A 126	6.35 7.28 7.24 5.70	7 43.60 3 46.25 4 46.52 8 45.88	1 28.352 4 27.943 6 30.375 1 29.733	1.00 1.00 1.00 1.00	0.26 0.00 0.00 0.00 0.00	C H H H
15	MOTA MOTA MOTA MOTA MOTA MOTA	2002 CA 2003 C 2004 O 2005 CB	LEU A 127 LEU A 127 LEU A 127 LEU A 127 LEU A 127	9.81 11.22	9 45.88 3 45.74 4 46.20 0 45.50	9 28.210 6 28.455 7 29.846 5 30.622		0.00 0.39 0.39 0.39	H N C C
20	ATOM ATOM ATOM ATOM ATOM	2007 CD1 2008 CD2 2009 H 2010 HA	LEU A 127 LEU A 127 LEU A 127 LEU A 127 LEU A 127	11.973 10.543 13.023 9.483 11.516	3 46.256 1 46.453 1 47.003 3 46.608	26.046 3 25.527 1 25.210 27.583	1.00 1.00 1.00 1.00	0.39 0.39 0.39 0.39	C C H
25	ATOM ATOM ATOM ATOM ATOM	2011 1HB 2012 2HB 2013 HG 2014 1HD1 2015 2HD1	LEU A 127 LEU A 127 LEU A 127 LEU A 127 LEU A 127	13.130 11.833 12.195 10.536 10.073	46.502 47.689 45.170 47.074	27.866 27.665 26.006 24.623	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H H
30	ATOM ATOM TOM ATOM ATOM	2016 3HD1 2017 1HD2 2018 2HD2 2019 3HD2	LEU A 127 LEU A 127 LEU A 127	9.942 12.582 13.035 14.037 11.008	47.094 46.866 48.076 46.592	26.169 24.252 25.442 25.281	1.00	0.00 0.00 0.00 0.00	н н н н
35	ATOM ATOM ATOM ATOM ATOM	2021 CA 2022 C 2023 O 2024 CB	LYS A 128 LYS A 128 LYS A 128 LYS A 128 LYS A 128	11.294 10.216 9.524 12.614 12.560	47.881 48.824 49.417 48.659	30.209 31.530 31.948 31.122 31.641	1.00 1.00 1.00 1.00	0.43 0.43 0.43 0.43	N C C C
40	ATOM ATOM ATOM ATOM ATOM	2026 CD 1 2027 CE 1 2028 NZ 1 2029 H 1	LYS A 128 LYS A 128 LYS A 128 LYS A 128 LYS A 128	13.718 13.540 12.447 10.328	50.948 52.388 53.031 47.889	30.960 31.350 30.872 31.635 29.646	1.00 (1.00 (1.00 (0.43 0.43 0.43 0.43 0.00	C C C N1+ H
45	ATOM ATOM ATOM ATOM ATOM	2031 1HB I 2032 2HB I 2033 1HG I 2034 2HG I	YS A 128 YS A 128 YS A 128 YS A 128 YS A 128	11.296 13.445 12.825 11.647 12.473	47.023 48.056 48.793 50.560 49.888	31.271	1.00 0 1.00 0 1.00 0	0.00 0.00 0.00 0.00	н н н н
50	ATOM ATOM ATOM ATOM ATOM	2036 2HD L 2037 1HE L 2038 2HE L 2039 1HZ L	YS A 128 YS A 128 YS A 128 YS A 128	14.667 13.841 13.239 14.468 12.368	50.553 50.944 52.423 52.924 54.022	32.449 29.841 31.072	1.00 0 1.00 0 1.00 0	.00 .00 .00 .00	н н н н
55	ATOM ATOM ATOM ATOM ATOM	2041 3HZ L 2042 N T 2043 CA T 2044 C T	YS A 128 YS A 128 YR A 129 YR A 129 YR A 129 YR A 129	11.541 12.593 10.043 9.095 9.784	52.625 52.977 48.960 49.877 50.604	32.634 33.275 33.832 34.940	1.00 0 1.00 0 1.00 0	.00 .00 .26 .26	H H N C
60	ATOM ATOM ATOM ATOM	2046 CB TY 2047 CG TY 2048 CD1 TY 2049 CD2 TY	TR A 129		50.160 51.165 50.051	34.435 1 35.325 1 34.823 1 36.687 1	.00 0.	.26 .26 .26 .26 .26	0 0 0 0 0
65	ATOM ATOM ATOM ATOM	2051 CE2 TY 2052 CZ TY 2053 OH TY 2054 H TY	R A 129 R A 129 R A 129 R A 129	6.707 5.916 5.283 10.608	50.930 51.931 52.830 48.473	37.540 1 37.035 1 37.916 1 33.952 1	.00 0.	26 26 26 26	C C O H
70	ATOM 2 ATOM 2	2056 1HB TY 2057 2HB TY 2058 HD1 TY	R A 129 R A 129 R A 129 R A 129 R A 129	8.174 4 7.213 4 6.455 5	50.575 48.298 48.793 51.455	33.049 1 35.013 1 33.637 1 33.799 1.	.00 0.0 .00 0.0 .00 0.0	00 1 00 1 00 1	H H H H

5	ATON ATON ATON ATON ATOM ATOM ATOM	4 2061 HE2 TYR A 12 4 2062 HH TYR A 12 5 2063 N TRP A 13 6 2064 CA TRP A 13 7 2065 C TRP A 13 8 2066 O TRP A 13	9 6.841 50.79 9 5.829 52.87 0 9.712 51.95 0 10.311 52.68 0 9.437 53.87	1 38.607 1.0 9 38.713 1.0 0 34.931 1.0 5 36.006 1.0 9 36.219 1.0	0 0.00 H 0 0.00 H 0 0.16 N 0 0.16 C 0 0.16 C
10	ATOM ATOM ATOM ATOM ATOM	2068 CG TRP A 13 2069 CD1 TRP A 13 2070 CD2 TRP A 13 2071 NE1 TRP A 13	0 11.716 53.211 0 12.467 53.739 0 12.409 54.960 0 13.463 52.984 0 13.299 55.007	35.683 1.0 36.882 1.0 37.486 1.0 37.588 1.0	0 0.16 C 0 0.16 C 0 0.16 C 0 0.16 C
15	MOTA MOTA MOTA MOTA MOTA MOTA MOTA	2073 CE3 TRP A 130 2074 CZ2 TRP A 130 2075 CZ3 TRP A 130 2076 CH2 TRP A 130	13.957 53.800 13.932 51.715 14.932 53.360 14.913 51.273 15.404 52.079	38.603 1.00 37.402 1.00 39.452 1.00 38.264 1.00	0 0.16 C 0 0.16 C 0 0.16 C 0 0.16 C
20	ATOM ATOM ATOM ATOM ATOM	2078 HA TRP A 130 2079 1HB TRP A 130 2080 2HB TRP A 130 2081 HD1 TRP A 130	10.329 52.061 11.622 53.988 12.306 52.403 11.643 55.612	34.292 1.00 36.916 1.00 34.909 1.00 35.220 1.00 37.343 1.00	0.00 H 0.00 H 0.00 H 0.00 H
25	ATOM ATOM ATOM ATOM ATOM	2083 HE3 TRP A 130 2084 HZ2 TRP A 130 2085 HZ3 TRP A 130 2086 HH2 TRP A 130	13.577 55.818 13.550 51.063 15.318 54.001 15.309 50.266 16.179 51.696	39.058 1.00 36.623 1.00 40.242 1.00 38.152 1.00 39.930 1.00	0.00 H 0.00 H 0.00 H
30	ATOM ATOM ATOM ATOM ATOM	2088 CA TYR A 131 2089 C TYR A 131 2090 O TYR A 131 2091 CB TYR A 131	9.204 54.267 8.351 55.401 8.991 56.631 8.436 57.284 8.087 55.714	37.487 1.00 37.683 1.00 37.120 1.00 36.238 1.00 39.164 1.00	0.17 N 0.17 C 0.17 C 0.17 O 0.17 O
35	ATOM ATOM ATOM ATOM ATOM	2093 CD1 TYR A 131 2094 CD2 TYR A 131 2095 CE1 TYR A 131 2096 CE2 TYR A 131	7.166 54.693 7.617 53.438 5.844 55.009 6.754 52.508 4.977 54.084	39.731 1.00 40.072 1.00 39.937 1.00 40.602 1.00 40.465 1.00	0.17 C 0.17 C 0.17 C 0.17 C 0.17 C
40	ATOM ATOM ATOM ATOM	2097 CZ TYR A 131 2098 OH TYR A 131 2099 H TYR A 131 2100 HA TYR A 131 2101 1HB TYR A 131	5.433 52.832 4.542 51.882 9.634 53.823 7.395 55.233 7.635 56.719	40.800 1.00 41.345 1.00 38.280 1.00 37.177 1.00 39.216 1.00	0.17 C 0.17 O 0.00 H 0.00 H
45	ATOM ATOM ATOM ATOM	2102 2HB TYR A 131 2103 HD1 TYR A 131 2104 HD2 TYR A 131 2105 HE1 TYR A 131 2106 HE2 TYR A 131	9.022 55.767 8.667 53.180 5.494 56.012 7.138 51.529 3.963 54.370	39.746 1.00 39.973 1.00 39.704 1.00 40.884 1.00 40.710 1.00	0.00 H 0.00 H 0.00 H
50	ATOM ATOM ATOM ATOM ATOM	2107 HH TYR A 131 2108 N GLU A 132 2109 CA GLU A 132 2110 C GLU A 132 2111 O GLU A 132	5.048 51.342 10.189 56.977 10.842 58.196 11.520 58.139	41.965 1.00 37.630 1.00 37.249 1.00 35.909 1.00	0.00 H 0.19 N 0.19 C 0.19 C
55	ATOM ATOM ATOM ATOM ATOM	2112 CB GLU A 132 2113 CG GLU A 132 2114 CD GLU A 132 2115 OE1 GLU A 132 2116 OE2 GLU A 132	11.851 58.705 13.030 57.774 13.838 58.387 14.098 59.618	38.295 1.00 38.565 1.00 39.702 1.00 39.651 1.00 40.641 1.00	0.19
60	ATOM	2117 H GLU A 132 2118 HA GLU A 132 2119 1HB GLU A 132 2120 2HB GLU A 132 2121 1HG GLU A 132	10.574 56.510 10.066 58.975 11.321 58.901 12.189 59.689 13.639 57.522	38.434 1.00 37.149 1.00 39.245 1.00 37.919 1.00	0.00 H 0.00 H 0.00 H 0.00 H 0.00 H
65	ATOM ATOM ATOM ATOM	2122 2HG GLU A 132 2123 N ASN A 133 2124 CA ASN A 133 2125 C ASN A 133 2126 O ASN A 133	12.498 56.967 3 12.116 56.988 3 12.974 56.963 3 12.209 57.009 3	39.059 1.00 35.539 1.00 34.382 1.00 33.098 1.00	0.00 H 0.18 N 0.18 C 0.18 C
70	ATOM ATOM	2127 CB ASN A 133 2128 CG ASN A 133 2129 OD1 ASN A 133 2130 ND2 ASN A 133	13.907 55.737 3 14.988 56.023 3 14.893 56.984 3	4.320 1.00 (3.284 1.00 (2.522 1.00 (0.18 C 0.18 C 0.18 C 0.18 O

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MOTA 2131 н ASN A 133 12.152 56.184 36.126 1.00 0.00 ATOM 2132 HA **ASN A 133** 57.843 13.641 34.482 1.00 MOTA 0.00 2133 1HB **ASN A 133** 13.387 54.810 34.048 1.00 0.00 ATOM 2134 2HB **ASN A 133** 14.388 55.588 5 35.302 1.00 0.00 ATOM 2135 1HD2 ASN A 133 54.411 16.149 33.904 1.00 0.00 MOTA 2136 2HD2 ASN A 133 16.735 55.326 32.538 1.00 0.00 MOTA 2137 N HIS A 134 12.358 58.148 32.393 1.00 0.16 ATOM 2138 CA HIS A 134 11.782 58.440 31.111 1.00 0.16 ATOM 2139 C HIS A 134 12.510 57.713 10 30.020 1.00 0.16 ATOM 2140 0 HIS A 134 11.908 57.336 29.016 1.00 0.16 MOTA 2141 HIS A 134 CB 11.845 59.939 30.781 1.00 0.16 ATOM 2142 CG HIS A 134 11.133 60.773 31.803 1.00 ND1 HIS A 134 0.16 ATOM 2143 9.767 60.954 31.837 1.00 0.16 ATOM 2144 CD2 HIS A 134 11.627 61.476 32.858 15 1.00 0.16 ATOM 2145 CE1 HIS A 134 9.506 61.751 32.903 1.00 0.16 MOTA 2146 NE2 HIS A 134 10.603 62.094 33.554 1.00 0.16 MOTA 2147 HIS A 134 H 12.816 58.920 32.852 1.00 0.00 ATOM 2148 HA HIS A 134 10.736 58.098 31.094 1.00 0.00 MOTA 2149 1HB HIS A 134 11.406 60.080 29.778 20 1.00 0.00 ATOM 2150 2HB HIS A 134 12.890 60.276 30.715 1.00 0.00 ATOM 2151 HD2 HIS A 134 12.657 61.578 33.175 1.00 0.00 MOTA 2152 HE1 HIS A 134 8.543 62.184 33.088 1.00 0.00 ATOM 2153 HE2 HIS A 134 10.667 62.639 34.389 1.00 0.00 ATOM 2154 **ASN A 135** N 13.835 57.507 25 30.179 1.00 0.14 ASN A 135 ATOM 2155 CA 14.631 56.982 29.100 1.00 0.14 ATOM 2156 C **ASN A 135** 14.941 55.534 29.306 1.00 MOTA 0.14 2157 0 **ASN A 135** 14.867 55.010 30.416 1.00 0.14 MOTA 2158 CB **ASN A 135** 15.986 57.690 28.963 1.00 0.14 ASN A 135 ATOM 2159 CG 15.720 59.156 30 28.665 1.00 0.14 MOTA 2160 OD1 ASN A 135 С 15.032 59.498 27.704 1.00 0.14 MOTA 2161 16.270 ND2 ASN A 135 60.053 29.528 1.00 0.14 ATOM 2162 H **ASN A 135** 14.277 57.581 31.090 1.00 0.00 H ATOM 2163 HA **ASN A 135** 57.126 14.091 28.156 1.00 0.00 MOTA 2164 1HB н ASN A 135 16.465 57.199 28.112 35 1.00 0.00 MOTA 2165 2HB H **ASN A 135** 16.609 57.530 29.857 1.00 0.00 MOTA 2166 1HD2 ASN A 135 16.809 59.763 30.324 1.00 0.00 ATOM 2167 2HD2 **ASN A 135** H 16.088 61.027 29.364 1.00 0.00 ATOM ILE A 136 н 2168 N 15.270 54.846 28.190 1.00 0.19 ATOM N 2169 CA ILE A 136 15.665 53.467 28.207 40 1.00 0.19 C ATOM 2170 С ILE A 136 16.831 53.341 27.279 1.00 ATOM 0.19 С 2171 0 ILE A 136 16.909 54.042 26.272 1.00 0.19 0 ATOM ILE A 136 2172 CB 14.612 52.529 27.694 1.00 0.19 C ATOM 2173 CG1 ILE A 136 15.014 51.070 27.966 1.00 0.19 MOTA ¢ 2174 14.381 CG2 ILE A 136 52.844 26.207 1.00 45 0.19 MOTA C 2175 CD1 ILE A 136 13.874 50.077 27.751 1.00 0.19 С MOTA 2176 H ILE A 136 15.312 55.307 27.283 1.00 0.00 ATOM H 2177 HA ILE A 136 15.976 53.214 29.234 1.00 0.00 ATOM 2178 HB ILE A 136 13.653 52.762 28.141 1.00 0.00 H 2179 1HG1 ILE A 136 MOTA 15.391 50.970 28.996 50 1.00 0.00 ATOM 2180 2HG1 ILE A 136 н 15.848 50.770 27.308 1.00 0.00 MOTA 2181 1HG2 ILE A 136 Н 13.544 52.256 25.812 1.00 MOTA 0.00 Н 2182 2HG2 ILE A 136 14.172 53.918 26.193 1.00 0.00 MOTA 2183 3HG2 ILE A 136 H 15.231 52.583 25.560 1.00 0.00 ATOM 2184 1HD1 ILE A 136 H 14.060 49.114 28.250 55 1.00 MOTA 0.00 Н 2185 2HD1 ILE A 136 12.927 50.491 28.101 1.00 0.00 H ATOM 2186 3HD1 ILE A 136 13.745 49.876 26.675 1.00 0.00 Н ATOM 2187 N **SER A 137** 17.788 52.452 27.604 1.00 0.24 ATOM N 2188 CA SER A 137 18.920 52.298 26.741 1.00 0.24 MOTA 2189 C **SER A 137** 19.203 50.837 26.610 60 1.00 0.24 C ATOM 2190 0 SER A 137 19.102 50.085 27.577 1.00 0.24 MOTA 2191 0 CB **SER A 137** 20.185 52.972 27.299 1.00 MOTA 2192 0.24 C OG **SER A 137** 21.276 52.795 26.411 1.00 0.24 MOTA 0 2193 H **SER A 137** 17.731 51.800 28.369 1.00 0.00 H ATOM 2194 SER A 137 HA 18.669 52.741 25.782 65 1.00 0.00 MOTA 2195 1HB H **SER A 137** 20.484 52.516 28.253 1.00 0.00 ATOM Н 2196 2HR **SER A 137** 20.000 54.044 27.484 1.00 0.00 ATOM H 2197 HG **SER A 137** 20.990 53.121 25.543 1.00 0.00 H ATOM 2198 ILE A 138 N 19.553 50.391 25.389 1.00 0.31 ATOM N 2199 CA ILE A 138 19.872 49.009 25.203 70 1.00 0.31 C ATOM 2200 С ILE A 138 21.299 48.973 24.779 1.00 0.31 ATOM C 2201 0 ILE A 138 21.688 49.613 23.804 1.00 0.31

5	OTA OTA OTA OTA	M 2203 CG1 ILE A 13 M 2204 CG2 ILE A 13 M 2205 CD1 ILE A 13	8 17.571 8 19.578 8 16.674	48.358 24.11 48.461 24.42 46.912 23.96 48.147 23.22	14 1.00 0.3 52 1.00 0.3	1 C
5	ATON ATON ATON ATON	M 2207 HA ILE A 13 M 2208 HB ILE A 13 M 2209 1HG1 ILE A 13	8 19.710 8 19.268 8 17.316	51.007 24.58 48.445 26.13 48.858 23.15 49.490 24.73	8 1.00 0.0 5 1.00 0.0 5 1.00 0.0 5 1.00 0.0	0 H 0 H 0 H
10	ATOM ATOM ATOM ATOM	2211 1HG2 ILE A 13: 2212 2HG2 ILE A 13: 2213 3HG2 ILE A 13: 2214 1HD1 ILE A 13:	8 18.854 8 20.505 8 19.788 15.696	47.817 25.28 46.237 23.49 46.865 23.36 46.455 24.94 48.643 23.34	2 1.00 0.0 9 1.00 0.0 4 1.00 0.0	0 H 0 H 0 H
15	MOTA MOTA MOTA MOTA MOTA	2216 3HD1 ILE A 136 2217 N THR A 139 2218 CA THR A 139	16.456 4 9 22.134 4 9 23.515 4	48.502 22.28 47.073 23.16 48.214 25.50 48.187 25.13	8 1.00 0.00 3 1.00 0.00 2 1.00 0.40 6 1.00 0.40	0 H 0 H 0 N
20	MOTA MOTA MOTA MOTA MOTA	2220 O THR A 139 2221 CB THR A 139 2222 OG1 THR A 139 2223 CG2 THR A 139	23.036 4 24.443 4 24.163 4 24.261 4	15.952 24.53 18.189 26.31 17.077 27.14 19.504 27.08	1.00 0.40 1 1.00 0.40 7 1.00 0.40)
25	ATOM ATOM ATOM ATOM	2224 H THR A 139 2225 HA THR A 139 2226 HB THR A 139 2227 HG1 THR A 139 2228 1HG2 THR A 139	23.767 4 25.487 4 24.393 4	17.655 26.299 19.068 24.524 18.132 25.945 16.277 26.647 19.573 27.923	1.00 0.00 1.00 0.00 1.00 0.00	H H H H
30	ATOM ATOM ATOM ATOM ATOM	2229 2HG2 THR A 139 2230 3HG2 THR A 139 2231 N ASN A 140 2232 CA ASN A 140	24.422 5 23.249 4 24.763 4 25.086 4	0.381 26.437 9.577 27.515 6.972 23.470 5.844 22.647	1.00 0.00 1.00 0.00 1.00 0.29	H H
35	ATOM ATOM ATOM ATOM	2233 C ASN A 140 2234 O ASN A 140 2235 CB ASN A 140 2236 CG ASN A 140 2237 OD1 ASN A 140	23.385 4 25.727 4 27.131 4 27.317 4	5.344 21.994 4.235 22.272 4.681 23.423 5.102 23.832 5.982 24.671	1.00 0.29 1.00 0.29 1.00 0.29 1.00 0.29 1.00 0.29	0000
40	ATOM ATOM ATOM ATOM ATOM	2238 ND2 ASN A 140 2239 H ASN A 140 2240 HA ASN A 140 2241 1HB ASN A 140 2242 2HB ASN A 140	25.351 4° 25.796 46 25.766 43	4.447 23.222 7.783 23.365 5.179 21.874 3.791 22.770 1.406 24.334	1.00 0.29 1.00 0.00 1.00 0.00 1.00 0.00	N H H H
45	MOTA MOTA MOTA MOTA MOTA MOTA	2243 1HD2 ASN A 140 2244 2HD2 ASN A 140 2245 N ALA A 141 2246 CA ALA A 141	27.995 43 29.087 44 23.250 46 22.029 45	3.721 22.547 1.710 23.487 3.167 21.107 1.798 20.453	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.26 1.00 0.26	H H H N C
50	MOTA MOTA MOTA MOTA	2247 C ALA A 141 2248 O ALA A 141 2249 CB ALA A 141 2250 H ALA A 141 2251 HA ALA A 141	23.383 44 21.490 46 23.587 47	.561 19.652 .293 19.206 .878 19.499 .104 20.927 .608 21.225	1.00 0.26 1.00 0.26 1.00 0.26 1.00 0.00	С С Н
55	ATOM ATOM ATOM	2252 1HB ALA A 141 2253 2HB ALA A 141 2254 3HB ALA A 141 2255 N THR A 142	20.549 46 21.267 47 22.201 47 21.198 43	.526 19.046 .806 20.048 .104 18.690 .763 19.475	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.35	H H H H N
	MOTA ATOM ATOM ATOM ATOM MOTA	2256 CA THR A 142 2257 C THR A 142 2258 O THR A 142 2259 CB THR A 142 2260 OG1 THR A 142	20.122 42 19.288 43 21.175 41	.535 18.746 .498 17.797 .401 17.779 .319 19.617	1.00 0.35 1.00 0.35 1.00 0.35 1.00 0.35	C C O C
60	MOTA MOTA MOTA MOTA	2261 CG2 THR A 142 2262 H THR A 142 2263 HA THR A 142 2264 HB THR A 142	19.764 41. 20.268 44. 22.202 42.	.145 18.859 .270 20.230 .072 19.709 .492 18.164 .382 20.430	1.00 0.35 1.00 0.35 1.00 0.00 1.00 0.00 1.00 0.00	О С Н Н
65	ATOM ATOM ATOM ATOM ATOM	2265 HG1 THR A 142 2266 1HG2 THR A 142 2267 2HG2 THR A 142 2268 3HG2 THR A 142 2269 N VAL A 143	20.924 39. 19.677 40. 19.545 42. 19.002 41.	425 19.314 455 20.966 189 20.799 155 19.495	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	н н н н
70	ATOM ATOM ATOM	2269 N VAL A 143 2270 CA VAL A 143 2271 C VAL A 143 2272 O VAL A 143	20.067 41. 19.038 41. 17.723 41. 16.696 41.		1.00 0.29 1.00 0.29 1.00 0.29 1.00 0.29	N C C O

	ATO:			.063 15.127	1.00 0.29) с
	ATO	M 2275 CG2 VAL A 14:		.966 14.122 .180 14.470	1.00 0.29	C
5	ATO	M 2276 H VALA 143	3 20.761 40	.180 14.470 .704 17.079	1.00 0.29 1.00 0.00	-
Ü	ATON ATON		18.850 42	.036 15.329	1.00 0.00	
	ATON	1320 27 17.		139 15.730	1.00 0.00	H
	ATOM	4 2280 2HG1 VAL A 143	17 142 20	173 13.377 710 14.609	1.00 0.00	H
10	ATOM	4 2281 3HG1 VAL A 143	17 962 40	710 14.609 905 13.559	1.00 0.00 1.00 0.00	H
10	ATOM ATOM		20.742 39.	540 13.578	1.00 0.00 1.00 0.00	H H
	ATOM			210 14.167	1.00 0.00	H
	ATOM		4	879 15.163 452 17.845	1.00 0.00	H
15	ATOM	2286 CA GLUA 144	16.522 40.		1.00 0.25	N
13	ATOM ATOM	020 11 144	15.953 41.		1.00 0.25 1.00 0.25	C C
	ATOM	C GHO V 144	14.738 41.	707 19.072	1.00 0.25	Ö
	ATOM	000 W 144	16.760 39. 17.200 37.		1.00 0.25	č
20	ATOM	2291 CD GLU A 144	17.200 37.9 18.626 38.0		1.00 0.25	С
20	ATOM	2292 OE1 GLU A 144	19.542 38.		1.00 0.25 1.00 0.25	C
	ATOM ATOM	2293 OE2 GLU A 144 2294 H GLU A 144	18.817 37.	791 17.849	1.00 0.25	0 01-
	MOTA	2294 H GLU A 144 2295 HA GLU A 144	18.487 39.6 15.773 39.6	18.039	1.00 0.00	Н
2.5	MOTA	2296 1HB GLU A 144	15.773 39.6 15.791 39.4		1.00 0.00	H
25	MOTA	2297 2HB GLU A 144	17.460 39.9	25 25	1.00 0.00 1.00 0.00	H
	ATOM ATOM	2298 1HG GLU A 144 2299 2HG GLU A 144	16.520 37.4	93 18.878	1.00 0.00	H H
	ATOM	2299 2HG GLU A 144 2300 N ASP A 145	17.181 37.4 16.834 42.5	02 20.537	1.00 0.00	H
30	MOTA	2301 CA ASP A 145	16.834 42.5 16.438 43.8		1.00 0.22	N
30	MOTA	2302 C ASP A 145	15.451 44.4		1.00 0.22 1.00 0.22	C
	ATOM ATOM	2303 O ASP A 145 2304 CB ASP A 145	14.495 45.0	69 19.079 1	1.00 0.22	C O
	ATOM	2304 CB ASP A 145 2305 CG ASP A 145	17.632 44.8 17.196 46.0	02 19.718 1	.00 0.22	č
25	ATOM	2306 OD1 ASP A 145	17.196 46.0 16.201 46.7		00 0.22	С
35	ATOM	2307 OD2 ASP A 145	17.856 46.4		.00 0.22	0
	ATOM ATOM	2308 H ASP A 145	17.800 42.4		.00 0.22	01- H
	ATOM	2309 HA ASP A 145 2310 1HB ASP A 145	15.940 43.74	45 20.598 1	.00 0.00	H
4.0	MOTA	2311 2HB ASP A 145	17.956 45.10 18.467 44.34		.00 0.00	H
40	ATOM	2312 N SER A 146	15.638 44.19		.00 0.00	H
	ATOM ATOM	2313 CA SER A 146 2314 C SER A 146	14.748 44.77		.00 0.20 .00 0.20	N C
	ATOM	2314 C SER A 146 2315 O SER A 146	13.344 44.38	4 16.696 1	.00 0.20	c
4.5	ATOM	2316 CB SER A 146	13.085 43.28 15.037 44.34		.00 0.20	0
45	ATOM	2317 OG SER A 146	14.798 42.95		.00 0.20 .00 0.20	C
	ATOM ATOM	2318 H SER A 146 2319 HA SER A 146	16.339 43.52		.00 0.20 .00 0.00	O H
	ATOM	2319 HA SER A 146 2320 1HB SER A 146	14.867 45.87	5 16.450 1.	00 0.00	H
50	ATOM	2321 2HB SER A 146	16.065 44.56 14.320 44.81	_	00 0.00	H
50	ATOM	2322 HG SER A 146	15.341 42.47	_	00 0.00	H
	MOTA MOTA	2323 N GLY A 147 2324 CA GLY A 147	12.394 45.30	5 16.442 1.	00 0.00 00 0.21	H N
	ATOM	2324 CA GLY A 147 2325 C GLY A 147	11.020 45.02	16.735 1.	00 0.21	Ĉ.
	ATOM	2326 O GLY A 147	10.301 46.33 10.814 47.349		00 0.21	С
55	ATOM	2327 H GLY A 147	12.612 46.212		00 0.21	0
	MOTA MOTA	2328 1HA GLY A 147 2329 2HA GLY A 147	10.941 44.526			H H
	ATOM	2329 2HA GLY A 147 2330 N THR A 148	10.566 44.365	15.975 1.		H
60	ATOM	2331 CA THR A 148	9.071 46.328 8.323 47.544			N
60		2332 C THR A 148	8.323 47.544 8.332 47.996			С
		2333 O THR A 148	8.106 47.205			C
		2334 CB THR A 148 2335 OG1 THR A 148	6.895 47.375	16.948 1.0		0
		2336 CG2 THR A 148	6.829 46.867	15.623 1.0		ō
65	ATOM	2337 H THR A 148	6.209 48.746 8.580 45.466	10	0.17	С
		2338 HA THR A 148	8.769 48.280	17.587 1.0 16.678 1.0		Н
		2339 HB THR A 148	6.366 46.654	16.678 1.0 17.589 1.0		H H
		2340 HG1 THR A 148 2341 1HG2 THR A 148	7.020 47.622	15.041 1.0		л Н
70	ATOM 2	2342 2HG2 THR A 148	5.151 48.632 6.285 49.123	16.730 1.0	0 0.00	H
	ATOM 2	2343 3HG2 THR A 148	6.285 49.123 6.671 49.461	18.038 1.0 16.318 1.0		H
			15.101	16.318 1.0	0 0.00	H

	ATON ATON	4 2345 CA TYR A 149		N C
	AOTA AOTA		7.643 50.872 20.494 1.00 0.12	C
5	ATON AOTA		7.419 51.669 19.586 1.00 0.12	0
	ATOM		11 045 40 000	C
	ATOM	I 2350 CD1 TYR A 149	13 674 40 000	C C
	ATOM ATOM		11.402 48.934 22.113 1.00 0.12	2
10	ATOM		12.644 47.904 19.899 1.00 0.12	3
	ATOM	2354 CZ TYR A 149	12 002 47 47	2
	ATOM	2355 OH TYR A 149	12.993 47.454 21.150 1.00 0.12 C	
	ATOM		8.800 49.943 18.247 1.00 0.00 H	
15	ATOM ATOM		8.441 48.967 21.010 1.00 0.00 H	
	ATOM		9.845 50.916 21.708 1.00 0.00 H 10.289 51.212 20.005 1.00 0.00 H	
	MOTA	2360 HD1 TYR A 149	11 401 40 211 12 751	
	ATOM		10.960 49.396 22.992 1.00 0.00 H	
20	MOTA MOTA		13.122 47.493 19.011 1.00 0.00 H	
	ATOM		13.003 48.093 23.120 1.00 0.00 H 14.639 46.549 20.554 1.00 0.00 H	
	ATOM	2365 N TYR A 150	6 000 FO 000	
	ATOM	2366 CA TYR A 150	6.072 51.960 21.976 1.00 0.12 C	
25	ATOM ATOM	2367 C TYR A 150 2368 O TYR A 150	6.183 52.188 23.446 1.00 0.12 C	
	ATOM	2368 O TYR A 150 2369 CB TYR A 150	6.750 51.369 24.169 1.00 0.12 0	
	MOTA	2370 CG TYR A 150	22:303 1:00 0:12	
	ATOM	2371 CD1 TYR A 150	3.990 50.559 22.220 1.00 0.12 C 3.295 50.653 23.419 1.00 0.12 C	
30	ATOM ATOM	2372 CD2 TYR A 150 2373 CE1 TYR A 150	4.191 49.295 21.666 1.00 0.12 C	
	ATOM	2373 CE1 TYR A 150 2374 CE2 TYR A 150	2.907 49.520 24.112 1.00 0.12 C	
	ATOM	2375 CZ TYR A 150	2 205	
	ATOM	2376 OH TYR A 150	3.066 47.123 24.350 1.00 0.12 0	
35	ATOM ATOM	2377 H TYR A 150 2378 HA TYR A 150	7.166 50.227 22.400 1.00 0.00 H	
	ATOM	2378 HA TYR A 150 2379 1HB TYR A 150	6.447 52.877 21.485 1.00 0.00 H 4.500 51.683 20.480 1.00 0.00 H	
	ATOM	2380 2HB TYR A 150	4 025 E2 C00 21 225	
	ATOM	2381 HD1 TYR A 150	3.054 51.631 23.829 1.00 0.00 H	
40	MOTA MOTA	2382 HD2 TYR A 150 2383 HE1 TYR A 150	4.684 49.206 20.701 1.00 0.00 H	
4.4	ATOM	2384 HE2 TYR A 150	2.366 49.635 25.050 1.00 0.00 H 3.992 47.177 21.897 1.00 0.00 H	
	ATOM	2385 HH TYR A 150	3.992 47.177 21.897 1.00 0.00 H 2.670 47.379 25.192 1.00 0.00 H	
	ATOM	2386 N CYS A 151	5.668 53.328 23.936 1.00 0.27 N	
45	ATOM ATOM	2387 CA CYS A 151 2388 C CYS A 151	5.851 53.607 25.325 1.00 0.27 C	
	ATOM	2389 O CYS A 151	4.536 53.997 25.912 1.00 0.27 C 3.648 54.482 25.215 1.00 0.27 O	
	ATOM	2390 CB CYS A 151	3.648 54.482 25.215 1.00 0.27 0 6.843 54.762 25.548 1.00 0.27 C	
	ATOM	2391 SG CYS A 151	7.171 55.139 27.291 1.00 0.27 S	
50	ATOM ATOM	2392 H CYS A 151 2393 HA CYS A 151	5.071 53.942 23.414 1.00 0.00 H	
	ATOM	2393 HA CYS A 151 2394 1HB CYS A 151	6.219 52.717 25.849 1.00 0.00 H 6.499 55.675 25.037 1.00 0.00 H	
	MOTA	2395 2HB CYS A 151	7 706 54 460 05 050	
	ATOM	2396 N THR A 152	4.373 53.738 27.222 1.00 0.37 N	
55	ATOM ATOM	2397 CA THR A 152 2398 C THR A 152	3.202 54.153 27.934 1.00 0.37 C	
	ATOM	2399 O THR A 152	3.659 54.946 29.104 1.00 0.37 C 4.747 54.733 29.635 1.00 0.37	
	MOTA	2400 CB THR A 152	4.747 54.733 29.635 1.00 0.37 0 2.327 53.042 28.434 1.00 0.37 C	
	MOTA	2401 OG1 THR A 152	3.105 52.054 29.091 1.00 0.37 0	
60	ATOM ATOM	2402 CG2 THR A 152 2403 H THR A 152	1.524 52.454 27.271 1.00 0.37 C	
	ATOM	2404 HA THR A 152	5.098 53.297 27.770 1.00 0.00 H 2.623 54.822 27.283 1.00 0.00 H	
	MOTA	2405 HB THR A 152	1 500 50 466 00 445 4 00 0.00 H	
	ATOM	2406 HG1 THR A 152	3.224 52.392 29.991 1.00 0.00 H	
65	MOTA MOTA	2407 1HG2 THR A 152	0.849 51.662 27.628 1.00 0.00 H	
	ATOM	2408 2HG2 THR A 152 2409 3HG2 THR A 152	0.960 53.241 26.770 1.00 0.00 H	
	ATOM	2410 N GLY A 153	2 920 55 010 00 700 4 44	
	ATOM	2411 CA GLY A 153	2.829 55.919 29.520 1.00 0.21 N 3.195 56.730 30.637 1.00 0.21 C	
70	ATOM ATOM	2412 C GLY A 153	1.974 57.474 31.040 1.00 0.21 C	
, 0	ATOM	2413 O GLY A 153 2414 H GLY A 153	1.021 57.588 30.271 1.00 0.21 0	
		H GHI M 103	1.886 56.034 29.142 1.00 0.00 H	

F	ATOM ATOM ATOM ATOM	2416 2HA 2417 N 2418 CA	GLY A 153 GLY A 153 LYS A 154 LYS A 154	3.54 1.97 0.80	3 56.101 2 58.006	31.450 32.275	1.00 0.0 1.00 0.0 1.00 0.1	0 H 2 N
5	MOTA ATOM ATOM ATOM ATOM	2420 O 2421 CB	LYS A 154 LYS A 154 LYS A 154 LYS A 154 LYS A 154	1.15 2.05 0.29 -0.17	5 60.151 9 60.530 0 58.265 6 56.810	32.821 33.565 34.077 34.106	1.00 0.1 1.00 0.1 1.00 0.1 1.00 0.1 1.00 0.1	2 C 2 O 2 C
10	MOTA MOTA MOTA MOTA MOTA	2424 CE 2425 NZ 2426 H 2427 HA 2428 1HB	LYS A 154 LYS A 154 LYS A 154 LYS A 154	-0.86 -1.04 2.73 0.03	3 54.818 6 54.378 3 57.898 1 58.632	35.521 35.557 36.959 32.935 31.958	1.00 0.12 1.00 0.12 1.00 0.00 1.00 0.00	C N1+
15	ATOM ATOM ATOM ATOM	2429 2HB 2430 1HG 2431 2HG 2432 1HD	LYS A 154 LYS A 154 LYS A 154 LYS A 154 LYS A 154	-0.526 1.176 0.548 -1.115 -1.072	58.355 56.156 56.752	34.362 34.684 33.586 33.543 36.083	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	H H H
20	ATOM ATOM ATOM ATOM ATOM	2433 2HD 2434 1HE 2435 2HE 2436 1HZ 2437 2HZ	LYS A 154 LYS A 154 LYS A 154 LYS A 154 LYS A 154	0.602 -0.129 -1.829 -1.436 -0.179	56.301 54.147 54.686 53.444	35.950 35.080 35.041 36.999 37.466	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	H H H
25	MOTA MOTA MOTA MOTA MOTA	2441 C	LYS A 154 VAL A 155 VAL A 155 VAL A 155 VAL A 155	-1.701 0.441 0.620 -0.646	54.977 60.994 62.404 62.882	37.445 32.056 32.171 32.782	1.00 0.00 1.00 0.00 1.00 0.20 1.00 0.20 1.00 0.20	H H C C
30	ATOM ATOM ATOM ATOM ATOM	2443 CB 2444 CG1 2445 CG2 2446 H	VAL A 155 VAL A 155 VAL A 155 VAL A 155	-1.735 0.804 2.117 -0.439 -0.465	62.479 63.105 62.612 62.853 60.701	30.854 30.221 29.983	1.00 0.20 1.00 0.20 1.00 0.20 1.00 0.20 1.00 0.00	о с с н
35	ATOM ATOM ATOM ATOM	2448 HB 2449 1HG1 2450 2HG1 2451 3HG1	/AL A 155 /AL A 155	1.474 0.898 2.526 2.861 1.975	62.627 64.185 63.319 62.443 61.644	32.829 31.070 29.484 31.007	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	н н н н
40	ATOM ATOM ATOM ATOM ATOM		AL A 155	-0.249 -0.649 -1.343 -0.539 -1.740	63.172 61.785 63.391 63.723	28.942 1 29.939 1 30.285 1 33.820 1	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.33	H H H H
45	ATOM ATOM ATOM ATOM ATOM	2457 C T 2458 O T 2459 CB T 2460 CG T	RP A 156 RP A 156 RP A 156 RP A 156 RP A 156	-2.323 -1.605 -2.765 -2.277	62.911 61.962 64.766 66.008	35.034 1 35.350 1 33.483 1 32.771 1	1.00 0.33 1.00 0.33 1.00 0.33 1.00 0.33 1.00 0.33	0000
50	ATOM ATOM ATOM ATOM ATOM	2462 CD2 T 2463 NE1 T 2464 CE2 T 2465 CE3 T	RP A 156 RP A 156 RP A 156 RP A 156 RP A 156	-1.694 -2.345 -1.392 -1.787 -2.832 -1.705	67.341 3 67.427 3 68.195 3 67.816 3	33.303 1 31.275 1 32.350 1 34.487 1	.00 0.33 .00 0.33 .00 0.33 .00 0.33	С С С
55	ATOM ATOM ATOM	2467 CZ3 T 2468 CH2 T 2469 H T 2470 HA T 2471 1HB T	RP A 156 RP A 156 RP A 156 RP A 156 RP A 156 RP A 156	-2.748 -2.195 0.348 -1.505 -3.617	69.175 3 70.021 3 64.062 3 64.859 3 65.114 3	4.703 1 3.763 1 4.155 1 5.270 1 4.092 1	.00 0.33 .00 0.33 .00 0.33 .00 0.00 .00 0.00	C C H H H
60	ATOM ATOM ATOM ATOM	2473 HD1 TF 2474 HE1 TF 2475 HE3 TF 2476 HZ2 TR	P A 156 P A 156 P A 156 P A 156	-1.470 -0.853 -3.265 -1.272	65.339 3 67.759 3 67.164 3 70.204 3	0.827 1. 0.508 1. 5.237 1. 1.826 1.	00 0.00 00 0.00 00 0.00 00 0.00 00 0.00	н н н н
65	ATOM 2 ATOM 2 ATOM 2 ATOM 2	2478 HH2 TR 2479 N GL 2480 CA GL 2481 C GL	P A 156 N A 157 N A 157 N A 157	-2.143 (-3.656 (-4.338 (-4.276 (71.087 3; 62.899 3; 51.769 3; 50.630 34	5.635 1. 3.972 1. 5.190 1. 5.739 1.	00 0.49 00 0.49	H H N C
70	ATOM 2	483 CB GLI 484 CG GLI	N A 157 N A 157	-5.830 6 -6.082 6	39.485 35 32.050 35 3.297 36	6.160 1.6 6.969 1.6 6.814 1.6 6.101 1.6	00 0.49 00 0.49 00 0.49	0000

```
ATOM
                     2486
                          OE1 GLN A 157
                                            -5.354
                                                     62.107 38.756 1.00
                                                                            0.49
              ATOM
                     2487
                           NE2 GLN A 157
                                            -4.525
                                                    64.203
                                                             38.466
                                                                     1.00
                                                                            0.49
              ATOM
                     2488
                           H
                                GLN A 157
                                            -4.225
                                                    63.687
                                                             34.941
              MOTA
                                                                     1.00
                                                                            0.00
                     2489
                                                                                    Н
                           HA
                               GLN A 157
                                            -3.849
                                                    61.453
     5
                                                             36.673
                                                                     1.00
                                                                           0.00
             ATOM
                     2490 1HB
                                                                                    H
                               GLN A 157
                                            -6.280
                                                    61.160
                                                            36.442
                                                                     1.00
                                                                           0.00
             ATOM
                     2491 2HB
                               GLN A 157
                                                                                    H
                                            -6.355
                                                    62.215
                                                            35.031
                                                                     1.00
             MOTA
                     2492
                                                                           0.00
                          1HG
                                                                                    H
                               GLN A 157
                                            -7.147
                                                    63.381
                                                            37.094
                                                                     1.00
             MOTA
                                                                           0.00
                     2493 2HG
                                                                                    H
                               GLN A 157
                                            -5.821
                                                    64.214
                                                            36.260
             MOTA
                                                                     1.00
                                                                           0.00
                     2494 1HE2 GLN A 157
                                                                                   H
                                            -4.495
   10
                                                    65.056
                                                            37.942
                                                                     1.00
                     2495 2HE2 GLN A 157
                                                                           0.00
             ATOM
                                                                                   H
                                            -3.997
                                                    64.103
                                                            39.316
                                                                    1.00
                                                                           0.00
             ATOM
                     2496
                          N
                               LEU A 158
                                           -4.459
                                                    60.932
                                                            33.473
             MOTA
                                                                    1.00
                                                                           0.41
                    2497
                                                                                   N
                          CA
                               LEU A 158
                                           -4.607
                                                    59.905
                                                           32.483
                                                                    1.00
             MOTA
                                                                           0.41
                    2498
                          С
                               LEU A 158
                                                                                   C
                                           -3.306
                                                    59.269
                                                           32.127
                                                                     1.00
             ATOM
                                                                           0.41
                    2499
                               LEU A 158
                                                                                   C
                          0
                                           -2.227
                                                    59.803
   15
                                                            32.381
                                                                    1.00
             ATOM
                    2500
                                                                           0.41
                          CB
                              LEU A 158
                                                                                   0
                                           -5.252
                                                    60.399
                                                            31.176
                                                                    1.00
             MOTA
                                                                           0.41
                    2501
                                                                                   C
                          CG
                              LEU A 158
                                           -6.699
                                                    60.889
                                                            31.364
                                                                    1.00
             MOTA
                                                                           0.41
                    2502
                          CD1 LEU A 158
                                                                                   C
                                           -7.628
                                                    59.742
             ATOM
                                                            31.796
                                                                    1.00
                                                                          0.41
                    2503
                          CD2
                              LEU A 158
                                                                                   C
                                           -6.758
                                                   62.101
                                                            32.310
                                                                    1.00
                                                                          0.41
             ATOM
                    2504
                          H
                              LEU A 158
                                                                                   C
                                           -4.372
   20
                                                   61.876
                                                            33.144
                                                                    1.00
             MOTA
                                                                          0.00
                    2505
                          HA
                              LEU A 158
                                                                                   H
                                           -5.247
                                                   59.120
                                                            32.926
            ATOM
                    2506 1HB
                                                                    1.00
                                                                          0.00
                                                                                   Н
                              LEU A 158
                                           -5.231
                                                   59.590
                                                            30.425
             ATOM
                                                                    1.00
                                                                          0.00
                    2507 2HB
                                                                                  H
                              LEU A 158
                                           -4.656
                                                   61.226
                                                           30.773
                                                                    1.00
            MOTA
                                                                          0.00
                    2508
                              LEU A 158
                                                                                  Н
                          HG
                                           -7.047
                                                   61.227
                                                           30.367
                                                                    1.00
            MOTA
                    2509 1HD1 LEU A 158
                                                                          0.00
                                                                                  H
                                           -8.682
                                                   60.066
  25
                                                           31.788
            ATOM
                    2510 2HD1 LEU A 158
                                                                    1.00
                                                                          0.00
                                                                                  H
                                          -7.548
                                                   58.883
                                                           31.108
                                                                    1.00
            ATOM
                                                                          0.00
                    2511 3HD1 LEU A 158
                                                                                  Н
                                          -7.408
                                                   59.385
            ATOM
                                                           32.814
                                                                    1.00
                                                                          0.00
                    2512 1HD2 LEU A 158
                                                                                  H
                                          -7.652
                                                   62.708
                                                           32.086
                                                                   1.00
            ATOM
                    2513 2HD2 LEU A 158
                                                                          0.00
                                                                                  H
                                          -6.896
                                                   61.750
                                                           33.331
            MOTA
                                                                   1.00
                                                                          0.00
                   2514 3HD2 LEU A 158
                                                                                  H
                                          -5.894
                                                   62.776
  30
                                                           32.222
                                                                   1.00
                                                                          0.00
            MOTA
                   2515
                                                                                  H
                         N
                              ASP A 159
                                          -3.419
                                                   58.062
                                                           31.533
            ATOM
                                                                   1.00
                                                                          0.19
                   2516
                             ASP A 159
                                                                                  N
                         CA
                                          -2.310
                                                  57.288
                                                           31.058
                                                                   1.00
            ATOM
                   2517
                                                                         0.19
                         С
                              ASP A 159
                                          -2.414
                                                  57.323
                                                           29.566
                                                                   1.00
            ATOM
                                                                         0.19
                   2518
                                                                                  C
                         0
                             ASP A 159
                                          -3.504
                                                  57.198
                                                           29.009
            MOTA
                                                                  1.00
                                                                         0.19
                   2519
                         CB
                             ASP A 159
                                                                                  0
  35
                                          -2.381
                                                  55.809
                                                           31.503
                                                                   1.00
            ATOM
                             ASP A 159
                                                                         0.19
                   2520
                                                                                  C
                         CG
                                          -1.124
                                                  55.027
                                                           31.117
                                                                   1.00
            MOTA
                   2521
                                                                         0.19
                         OD1 ASP A 159
                                                                                  C
                                          -0.378
                                                  55.468
                                                          30.205
           ATOM
                                                                   1.00
                                                                         0.19
                   2522
                         OD2 ASP A 159
                                                                                  0
                                          -0.904
                                                  53.956
                                                          31.744
                                                                   1.00
           ATOM
                                                                         0.19
                                                                                 01
                   2523
                         H
                             ASP A 159
                                          -4.304
                                                  57.666
                                                          31.271
                                                                  1.00
           ATOM
                                                                         0.00
                   2524
                             ASP A 159
                                                                                 H
                         HA
                                          -1.394
                                                  57.724
  40
                                                          31.412
                                                                   1.00
                                                                         0.00
           ATOM
                   2525 1HB
                                                                                 H
                             ASP A 159
                                         -3.242
                                                  55.320
                                                          31.016
                                                                  1.00
           ATOM
                  2526 2HB
                                                                         0.00
                                                                                 H
                             ASP A 159
                                         -2.577
                                                  55.702
                                                          32.580
                                                                  1.00
                                                                         0.00
           ATOM
                  2527
                                                                                 H
                        N
                             TYR A 160
                                         -1.279 57.531
                                                          28.874
           ATOM
                                                                   1.00
                                                                         0.11
                  2528
                             TYR A 160
                                                                                 N
                        CA
                                         -1.321
                                                 57.584
                                                          27.443
                                                                  1.00
                                                                         0.11
           ATOM
                  2529
                                                                                 C
                        C
                             TYR A 160
                                         -0.381
 45
                                                 56.562
                                                          26.901
                                                                  1.00
           ATOM
                                                                         0.11
                  2530
                                                                                 C
                        0
                             TYR A 160
                                         0.535
                                                 56.111
                                                          27.589
           ATOM
                                                                  1.00
                                                                         0.11
                                                                                 0
                  2531
                        CB
                             TYR A 160
                                         -0.884
                                                 58.937
                                                          26.857
                                                                  1.00
                                                                         0.11
           ATOM
                                                                                 C
                  2532
                        CG
                             TYR A 160
                                         -1.939
                                                 59.942
                                                          27.171
                                                                  1.00
           ATOM
                  2533
                                                                         0.11
                                                                                 C
                        CD1 TYR A 160
                                         -2.067
                                                 60.462
                                                         28.439
                                                                  1.00
           ATOM
                  2534
                                                                        0.11
                                                                                 C
                        CD2 TYR A 160
                                         -2.794
                                                 60.378
                                                         26.185
 50
           MOTA
                                                                  1.00
                                                                        0.11
                                                                                 C
                  2535
                        CE1
                            TYR A 160
                                         -3.042
                                                 61.390
                                                         28.720
                                                                  1.00
                                                                        0.11
          ATOM
                                                                                 C
                  2536
                        CE2 TYR A 160
                                         -3.771
                                                 61.306
                                                         26.459
                                                                  1.00
                                                                        0.11
          ATOM
                  2537
                        CZ
                                                                                 C
                            TYR A 160
                                         -3.895
                                                 61.814
                                                         27.730
          ATOM
                                                                  1.00
                                                                        0.11
                  2538
                                                                                 C
                        OH
                            TYR A 160
                                         -4.895
                                                 62.767
                                                         28.019
                                                                  1.00
          MOTA
                                                                        0.11
                                                                                 0
                  2539
                        H
                            TYR A 160
                                        -0.429
                                                 57.158
 55
                                                         29.312
                                                                  1.00
                                                                        0.00
          ATOM
                  2540
                        HA
                            TYR A 160
                                                                                H
                                         -2.323
                                                 57.325
                                                         27.087
                                                                  1.00
                                                                        0.00
          ATOM
                 2541 1HB
                            TYR A 160
                                         -0.756
                                                 58.828
                                                         25.769
                                                                 1.00
          MOTA
                 2542
                                                                        0.00
                                                                                H
                       2HB
                            TYR A 160
                                        0.099
                                                 59.231
                                                         27.261
                                                                 1.00
                                                                        0.00
          ATOM
                 2543
                       HD1 TYR A 160
                                                                                H
                                        -1.420
                                                 60.088
                                                         29.225
                                                                 1.00
                                                                        0.00
          MOTA
                 2544
                       HD2 TYR A 160
                                                                                Н
                                        -2.708
                                                59.975
60
                                                        25.179
                                                                 1.00
                                                                        0.00
          MOTA
                 2545
                       HE1 TYR A 160
                                                                                H
                                        -3.087
                                                 61.827
                                                         29.711
                                                                 1.00
                 2546
                                                                        0.00
          MOTA
                                                                                H
                       HE2 TYR A 160
                                        -4.440
                                                 61.623 25.662
                                                                        0.00
                                                                 1.00
          ATOM
                 2547
                       HH TYR A 160
                                                                                Н
                                        -5.696
                                                62.470
                                                         27.566
                                                                 1.00
                                                                       0.00
          ATOM
                 2548
                                                                                H
                       N
                            GLU A 161
                                        -0.622
                                                56.144
                                                         25.643
                                                                 1.00
          MOTA
                 2549
                                                                       0.12
                                                                                N
                       CA
                           GLU A 161
                                         0.262
                                                55.219
                                                         25.000
65
                                                                 1.00
         MOTA
                                                                       0.12
                 2550
                                                                                C
                       C
                           GLU A 161
                                         0.753
                                                55.893
                                                         23.762
                                                                 1.00
                                                                       0.12
         ATOM
                 2551
                                                                                C
                       0
                           GLU A 161
                                         0.033
                                                56.669
                                                         23.135
                                                                 1.00
         ATOM
                                                                       0.12
                 2552
                                                                                0
                       CB
                           GLU A 161
                                        -0.537
                                                53.970
                                                        24.530
                                                                 1.00
                                                                       0.12
         MOTA
                                                                                C
                 2553
                           GLU A 161
                       CG
                                        -1.765
                                                53.494
                                                        25.343
                                                                 1.00
         ATOM
                                                                       0.12
                                                                                C
                 2554
                           GLU A 161
                       CD
                                        -1.424
                                                52.544
70
                                                        26.509
                                                                 1.00
                                                                       0.12
                2555
         MOTA
                                                                               C
                       OE1 GLU A 161
                                        -1.294
                                                51.360
                                                        26.186
                                                                 1.00
                                                                       0.12
                                                                               0
         MOTA
                2556
                      OE2 GLU A 161
                                        -1.270
                                                53.072
                                                        27.616
                                                                 1.00
                                                                       0.12
```

	ATOM ATOM ATOM	2558 на	GLU A 161 GLU A 161 GLU A 161	1.08	2 54.949	25.66	1.00	0.00	н
5	ATOM ATOM ATOM	2560 2HB 2561 1HG 2562 2HG	GLU A 161 GLU A 161 GLU A 161	-0.92° -2.415 -2.358	7 54.220 5 52.932 8 54.344	23.53 24.65 25.709	l 1.00 l 1.00	0.00	H H H
10	ATOM ATOM ATOM	2564 CA 2565 C	SER A 162 SER A 162 SER A 162 SER A 162	2.020 2.598 2.381 1.967	56.250 55.367	22.242	1.00	0.11 0.11 0.11	N C C
	ATOM ATOM ATOM	2568 OG 2569 H	SER A 162 SER A 162 SER A 162	4.113 4.614 2.604	56.489 57.110 55.025	22.371 21.196	1.00	0.11 0.11 0.11 0.00	о С О
15	MOTA MOTA MOTA MOTA	2571 1HB	SER A 162 SER A 162 SER A 162 SER A 162	2.118 4.627 4.316 5.577	55.527 57.117	22.518	1.00 1.00	0.00 0.00 0.00 0.00	H H H
20	MOTA MOTA MOTA MOTA	2574 N 2575 CA 2576 C 2577 O	GLU A 163 GLU A 163 GLU A 163 GLU A 163	2.640 2.517 3.757	55.915 55.151 54.333	19.864 18.661 18.544	1.00 1.00 1.00	0.13 0.13 0.13	H N C C
25	ATOM ATOM ATOM	2578 CB 2579 CG 2580 CD	GLU A 163 GLU A 163 GLU A 163	4.830 2.382 3.567 3.153	54.718 56.031 56.976 58.020	19.006 17.407 17.202 16.177	1.00 1.00 1.00	0.13 0.13 0.13 0.13	0 0 0 0
25	ATOM ATOM ATOM ATOM		GLU A 163 GLU A 163 GLU A 163 GLU A 163	2.076 3.900 3.159 1.565	58.643 58.212 56.782 54.603	16.381 15.181 19.804 18.736	1.00 1.00 1.00	0.13 0.13 0.00	0 01- H
30	MOTA ATOM ATOM ATOM	2585 1HB 2586 2HB 2587 1HG 2588 2HG	GLU A 163 GLU A 163 GLU A 163 GLU A 163	1.438 2.265 4.481 3.766	56.596 55.357 56.445	17.501 16.540 16.900	1.00 1.00 1.00	0.00 0.00 0.00	H H H
35	MOTA MOTA TOM ATOM	2589 N 2590 CA 2591 C	PRO A 164 PRO A 164 PRO A 164	3.611 4.751 5.680	57.518 53.185 52.324 52.796	18.137 17.956 17.819 16.752	1.00 1.00 1.00 1.00	0.00 0.13 0.13 0.13	H N C C
40	ATOM ATOM ATOM	2593 CB 2594 CG 2595 CD	PRO A 164 PRO A 164 PRO A 164 PRO A 164	5.235 4.189 2.815 2.385	53.459 50.930 50.957 52.429	15.818 17.565 18.251 18.167	1.00 1.00 1.00 1.00	0.13 0.13 0.13 0.13	0 0 0
40	ATOM ATOM ATOM ATOM	2597 1HB 2598 2HB	PRO A 164 PRO A 164 PRO A 164 PRO A 164	5.289 4.769 4.113 2.920	52.312 50.185 50.690 50.648	18.774 18.092 16.495	1.00 1.00 1.00	0.00 0.00 0.00	H H H
45	ATOM ATOM ATOM	2600 2HG 2601 1HD 2602 2HD	PRO A 164 PRO A 164 PRO A 164	2.075 1.700 1.875	50.275 52.602 52.702	19.303 17.803 17.322 19.099	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H H
50	ATOM ATOM ATOM ATOM ATOM	2604 CA 2605 C 2606 O	LEU A 165 LEU A 165 LEU A 165 LEU A 165 LEU A 165	6.982 7.932 8.678 8.896	52.483 52.840 51.587 50.754	16.888 15.879 15.565 16.444	1.00 1.00 1.00 1.00	0.11 0.11 0.11 0.11	N C C
55	ATOM ATOM ATOM ATOM	2608 CG 1 2609 CD1 1 2610 CD2 1	LEU A 165 LEU A 165 LEU A 165 LEU A 165	8.953 8.309 9.377 7.321	53.897 55.248 56.304 55.708	16.327 16.688 17.011 15.605	1.00 1.00 1.00	0.11 0.11 0.11 0.11	с с с
	ATOM ATOM ATOM	2612 HA 1 2613 1HB 1 2614 2HB 1	LEU A 165 LEU A 165 LEU A 165	7.333 7.399 9.663 9.540	52.020 53.174 54.039 53.512	17.718 14.975 15.492 17.180	1.00	0.00 0.00 0.00 0.00	Н Н Н
60	ATOM ATOM ATOM ATOM	2616 1HD1 I 2617 2HD1 I 2618 3HD1 I	EU A 165 EU A 165	10.045	55.959 56.456	16.150	1.00 (1.00 (1.00 (0.00 0.00 0.00	H H H
65	ATOM ATOM ATOM ATOM ATOM		EU A 165	7.617 6.293 9.077	55.405 55.405 51.402	15.620 14.591 15.796 14.294	1.00 0 1.00 0 1.00 0	0.00 0.00 0.00 0.10	H H H N
70	ATOM ATOM ATOM ATOM	2624 C A 2625 O A 2626 CB A	SN A 166	11.234 11.729 9.460	50.478 51.346 49.623	14.008 13.291 12.581	1.00 0 1.00 0 1.00 0	.10 .10 .10 .10	00000

5	ATOM ATOM ATOM ATOM ATOM ATOM	2629 ND2 ASN A 1	66 7.695 66 8.934 66 9.513 66 10.186	48.328 11. 52.059 13. 49.396 14. 48.815 12.	555 1.00 0.1 490 1.00 0.1 548 1.00 0.06 694 1.00 0.06 378 1.00 0.06	0 N 0 H 0 H
10	ATOM ATOM ATOM ATOM ATOM	2634 1HD2 ASN A 10 2635 2HD2 ASN A 10 2636 N ILE A 10 2637 CA ILE A 10 2638 C ILE A 10 2639 O ILE A 10	56 8.315 56 6.774 57 11.959 57 13.378 57 13.954 57 13.535	50.379 11. 48.199 10. 47.924 11. 49.747 14. 49.904 14. 48.591 14.: 47.544 15.:	489 1.00 0.00 873 1.00 0.22 942 1.00 0.22 545 1.00 0.22	H H C C
15	ATOM ATOM ATOM ATOM ATOM	2640 CB ILE A 16 2641 CG1 ILE A 16 2642 CG2 ILE A 16 2643 CD1 ILE A 16 2644 H ILE A 16	7 13.880 7 13.316 7 15.418 7 13.532 7 11.571	50.216 16.3 51.562 16.8 50.161 16.3 51.815 18.3 48.981 15.4	322 1.00 0.22 305 1.00 0.22 294 1.00 0.22 297 1.00 0.22	0 0 0
20	ATOM ATOM ATOM ATOM ATOM	2645 HA ILE A 16 2646 HB ILE A 16 2647 1HG1 ILE A 16 2648 2HG1 ILE A 16 2649 1HG2 ILE A 16	7 13.699 7 13.530 7 12.227 7 13.758 7 15.829	50.705 14.2 49.426 17.0 51.610 16.6 52.388 16.2	61 1.00 0.00 14 1.00 0.00 23 1.00 0.00 19 1.00 0.00	н н н н
25	ATOM ATOM ATOM ATOM ATOM	2650 2HG2 ILE A 16 2651 3HG2 ILE A 16 2652 1HD1 ILE A 16 2653 2HD1 ILE A 16 2654 3HD1 ILE A 16	7 15.817 7 15.852 7 13.012 7 13.158	49.186 15.9 50.951 15.6 52.730 18.6 50.981 18.9	76 1.00 0.00 70 1.00 0.00 21 1.00 0.00 09 1.00 0.00	н н н н
30	ATOM ATOM ATOM ATOM ATOM	2655 N THR A 168 2656 CA THR A 168 2657 C THR A 168 2658 O THR A 168 2659 CB THR A 168	14.926 15.488 16.955 17.587	51.943 18.5 48.604 13.6 47.353 13.2 47.396 13.4 48.447 13.3	18 1.00 0.48 12 1.00 0.48 10 1.00 0.48 12 1.00 0.48	H N C C O
35	ATOM ATOM ATOM ATOM ATOM	2660 OG1 THR A 168 2661 CG2 THR A 168 2662 H THR A 168 2663 HA THR A 168 2664 HB THR A 168	15.798 13.800 15.334 15.086	47.020 11.76 48.064 10.94 46.788 11.49 49.451 13.24 46.551 13.82	18 1.00 0.48 94 1.00 0.48 12 1.00 0.00	С С Н Н
40	ATOM ATOM ATOM ATOM	2665 HG1 THR A 168 2666 1HG2 THR A 168 2667 2HG2 THR A 168 2668 3HG2 THR A 168	16.752 13.629 13.392 13.218	46.078 11.54 48.111 11.10 46.488 10.44 45.995 12.14 47.707 11.67	7 1.00 0.00 7 1.00 0.00 1 1.00 0.00	н н н н
45	ATOM ATOM ATOM ATOM	2670 CA VAL A 169 2671 C VAL A 169 2672 O VAL A 169 2673 CB VAL A 169	18.958 19.375 18.935	46.228 13.72 46.199 13.79 45.828 12.41 44.820 11.86 45.207 14.77	4 1.00 0.55 5 1.00 0.55 5 1.00 0.55 3 1.00 0.55	N C C O
50	ATOM ATOM ATOM ATOM	2674 CG1 VAL A 169 2675 CG2 VAL A 169 2676 H VAL A 169 2677 HA VAL A 169 2678 HB VAL A 169	19.096 4 19.102 4 17.097 4 19.344 4	15.621 16.18 13.782 14.39 15.329 13.64 17.190 14.06 15.296 14.67	3 1.00 0.55 1 1.00 0.55 3 1.00 0.00 9 1.00 0.00	C C H H
55	ATOM 2 ATOM 2 ATOM 2 ATOM 2	2679 1HG1 VAL A 169 2680 2HG1 VAL A 169 2681 3HG1 VAL A 169 2682 1HG2 VAL A 169 2683 2HG2 VAL A 169	19.882 4 18.919 4 18.150 4 19.961 4 18.107 4	5.432 16.925 6.708 16.250 5.151 16.482 3.256 14.838 3.608 14.822	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	н н н н н
60	ATOM 2 ATOM 2 ATOM 2 ATOM 2	2684 3HG2 VAL A 169 2685 N ILE A 170 2686 CA ILE A 170 2687 C ILE A 170 2688 O ILE A 170 2689 CB ILE A 170	20.221 40 20.637 40 21.357 41 21.198 44	3.378 13.385 6.672 11.807 6.451 10.457 5.145 10.428 4.364 9.490	1.00 0.00 1.00 0.56 1.00 0.56 1.00 0.56 1.00 0.56	H C C C
65	ATOM 2 ATOM 2 ATOM 2 ATOM 2	690 CG1 ILE A 170 691 CG2 ILE A 170 692 CD1 ILE A 170 693 H ILE A 170	21.728 47 22.867 47 22.467 46	7.545 9.942 7.467 8.414 7.492 10.727 5.223 7.921 7.485 12.272	1.00 0.56 1.00 0.56 1.00 0.56 1.00 0.56	С С С
70	ATOM 26 ATOM 26 ATOM 26	694 HA ILE A 170 695 HB ILE A 170 696 1HG1 ILE A 170 697 2HG1 ILE A 170 698 1HG2 ILE A 170	19.739 46 21.142 48 22.296 48 20.748 47	349 9.824 .513 10.164 .360 8.094 .543 7.909 .524 10.855	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	н н н н н

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MOTA
                     2699 2HG2 ILE A 170
                                            22.796
                                                     47.047
                                                             11.714 1.00 0.00
                     2700 3HG2 ILE A 170
              ATOM
                                            23.675
                                                     46.954
                                                             10.210
                                                                      1.00
                                                                            0.00
             ATOM
                     2701 1HD1 ILE A 170
                                            23.115
                                                     46.497
                                                              7.070
                                                                     1.00
                                                                            0.00
             ATOM
                                                                                    H
                     2702 2HD1 ILE A 170
                                            23.131
                                                     45.742
     5
                                                              8.651
                                                                     1.00
                                                                            0.00
             MOTA
                     2703 3HD1 ILE A 170
                                                                                    H
                                            21.776
                                                     45.472
                                                              7.510
                                                                     1.00
                                                                            0.00
             MOTA
                     2704
                                                                                    H
                               LYS A 171
                          N
                                            22.156
                                                    44.867
                                                             11.475
                                                                     1.00
             MOTA
                                                                            0.52
                     2705
                                                                                    N
                           CA
                              LYS A 171
                                            22.902
                                                    43.646
                                                             11.537
                                                                     1.00
                                                                            0.52
             ATOM
                     2706
                               LYS A 171
                                                                                    C
                           С
                                            21.908
                                                    42.536
                                                             11.406
                                                                     1.00
                                                                            0.52
             ATOM
                     2707
                                                                                    C
                           0
                               LYS A 171
                                            20.957
                                                    42.448
   10
                                                             12.180
                                                                     1.00
                                                                           0.52
             ATOM
                     2708
                          CB
                               LYS A 171
                                                                                    0
                                            23.649
                                                    43.510
                                                             12.879
                                                                     1.00
             MOTA
                                                                           0.52
                    2709
                          CG
                               LYS A 171
                                            24.731
                                                    42.430
                                                            12.935
                                                                     1.00
                                                                           0.52
             ATOM
                    2710
                                                                                    C
                          CD
                               LYS A 171
                                            24.206
                                                    41.006
                                                            12.790
                                                                     1.00
                                                                           0.52
             ATOM
                               LYS A 171
                                                                                    C
                    2711
                           CE
                                            25.263
                                                    39.934
                                                            13.064
                                                                     1.00
                                                                           0.52
             MOTA
                    2712
                               LYS A 171
                                                                                    C
                          NZ
                                            26.436
                                                    40.153
   15
                                                            12.190
                                                                     1.00
             ATOM
                                                                           0.52
                    2713
                                                                                    N1+
                          Н
                               LYS A 171
                                           22.064
                                                    45.419
                                                            12.309
                                                                     1.00
                                                                           0.00
             ATOM
                                                                                    н
                    2714
                          HA
                               LYS A 171
                                           23.632
                                                    43.648
                                                            10.707
                                                                     1.00
             ATOM
                                                                           0.00
                    2715 1HB
                               LYS A 171
                                                                                    H
                                           22.872
                                                    43.341
                                                            13.643
                                                                     1.00
                                                                           0.00
             MOTA
                    2716 2HB
                                                                                    H
                               LYS A 171
                                           24.129
                                                    44.479
                                                            13.070
                                                                     1.00
                                                                           0.00
             ATOM
                    2717 1HG
                                                                                    H
                               LYS A 171
                                           25.345
                                                    42.498
  20
                                                            13.836
                                                                    1.00
                                                                           0.00
             MOTA
                    2718 2HG
                                                                                   Н
                              LYS A 171
                                           25.440
                                                    42.623
                                                            12.108
            ATOM
                                                                    1.00
                                                                           0.00
                              LYS A 171
LYS A 171
                                                                                   Н
                    2719 1HD
                                           23.964
                                                    40.933
                                                            11.730
                                                                    1.00
                                                                           0.00
            MOTA
                    2720 2HD
                                                                                   H
                                           23.302
                                                    40.816
                                                            13.390
                                                                    1.00
                                                                          0.00
            MOTA
                                                                                   H
                    2721 1HE
                              LYS A 171
                                           24.877
                                                   38.923
                                                            12.853
                                                                    1.00
                                                                           0.00
            ATOM
                    2722 2HE
                                                                                   H
                              LYS A 171
                                           25.630
27.152
                                                   39.937
  25
                                                            14.101
            MOTA
                                                                    1.00
                                                                          0.00
                                                                                   Н
                    2723 1HZ
                              LYS A 171
                                                   39.454
                              LYS A 171
LYS A 171
                                                            12.333
                                                                    1.00
                                                                          0.00
            ATOM
                    2724
                        2HZ
                                                                                   H
                                           26.174
                                                   40.112
                                                            11.214
                                                                    1.00
                                                                          0.00
            ATOM
                    2725 3HZ
                                                                                   Н
                                           26.861
                                                   41.053
                                                            12.366
                                                                    1.00
            ATOM
                                                                          0.00
                   2726
                                                                                   H
                         N
                              ALA A 172
                                           22.097
                                                   41.667
                                                            10.393
                                                                    1.00
                                                                          0.31
            ATOM
                                                                                   N
                   2727
                          CA
                              ALA A 172
                                           21.148
                                                   40.617
                                                            10.164
  30
                                                                    1.00
            ATOM
                                                                          0.31
                                                                                   C
                   2728
                          С
                              ALA A 172
                                          21.773
                                                   39.272
                                                            10.514
                                                                    1.00
                                                                          0.31
                              ALA A 172
            MOTA
                   2729
                                                                                   C
                         0
                                           21.353
                                                   38.260
                                                            9.895
                                                                    1.00
            MOTA
                                                                          0.31
                   2730
                         CB
                              ALA A 172
                                          20.692
                                                   40.524
                                                            8.698
                                                                    1.00
                                                                          0.31
            ATOM
                                                                                   C
                   2731
                         OXT ALA A 172
                                          22.663
                                                   39.229
                                                           11.402
                                                                   1.00
                                                                          0.31
            MOTA
                   2732
                                                                                   01
                         H
                              ALA A 172
                                          22.807
                                                   41.776
  35
                                                            9.698
                                                                    1.00
                                                                          0.00
            MOTA
                   2733
                                                                                  H
                         HA
                             ALA A 172
                                          20.252
                                                   40.765
                                                           10.785
                                                                   1.00
                                                                          0.00
            MOTA
                   2734 1HB
                                                                                   Н
                              ALA A 172
                                          19.857
                                                  39.810
                                                            8.602
                                                                   1.00
                                                                          0.00
           ATOM
                   2735 2HB
                             ALA A 172
                                                                                  H
                                          20.320
                                                  41.491
                                                            8.321
                                                                          0.00
                                                                   1.00
                             ALA A 172
           ATOM
                                                                                  H
                   2736 3HB
                                          21.505
                                                  40.199
                                                            8.030
                                                                   1.00
                                                                          0.00
           ATOM
                   2737 N
                             VAL B 1
                                                                                  H
                                         -35.035
                                                  33.443
 40
                                                           -3.312
                                                                   1.00
                                                                          0.14
           MOTA
                   2738 CA
                                                                                  N1
                             VAL B
                                         -36.312
                                                  33.784
                                                           -2.644
                                                                   1.00
           MOTA
                   2739 C
                                                                          0.14
                                                                                  C
                                    1 -36.557
                             VAL B
                                                  33.129
                                                           -1.314
                                                                   1.00
           ATOM
                                                                          0.14
                                                                                  C
                  2740
                                    1 -37.357
1 -37.484
                         0
                             VAL B
                                                  33.653
                                                          -0.542
                                                                   1.00
                                                                          0.14
           ATOM
                                                                                  0
                  2741
                         CB
                             VAL B
                                                  33.539
                                                           -3.566
                                                                   1.00
                                                                         0.14
           MOTA
                                                                                  С
                  2742
                         CG1 VAL B
                                    1 -37.364
                                                  34.515
                                                          -4.747
 45
                                                                   1.00
                  2743
                                                                         0.14
           ATOM
                                                                                  C
                         CG2 VAL B
                                     1 -37.528
                                                  32.067
                                                           -4.005
           ATOM
                                                                   1.00
                                                                         0.14
                                                                                  С
                  2744 1H
                             VAL B
                                     1 -34.869
                                                  34.004
                                                          -4.138
                                                                   1.00
                                                                         0.00
                  2745 2H
                                                                                  H
           ATOM
                             VAL B
                                     1 -34.241
                                                  33.598
                                                          -2.703
                                                                   1.00
                                                                         0.00
           MOTA
                  2746 3H
                                                                                  Н
                             VAL B
                                        -34.995
                                     1
                                                          -3.602
                                                  32.476
                                                                   1.00
           MOTA
                                                                         0.00
                                                                                  Н
                  2747
                        HA
                             VAL B
                                     1 -36.235
                                                  34.860
                                                          -2.400
 50
                                                                   1.00
                                                                         0.00
           ATOM
                                                                                  н
                  2748
                        HB
                             VAL B
                                     1
                                        -38.411
                                                  33.777
                                                          -3.011
                                                                   1.00
                                                                         0.00
           MOTA
                  2749 1HG1 VAL B
                                                                                 Н
                                     1
                                        -38.229
                                                  34.435
                                                          -5.429
                                                                   1.00
                                                                         0.00
           MOTA
                  2750 2HG1 VAL B
                                                                                 H
                                       -37.326
                                                 35.564
                                                          -4.406
                                                                  1.00
                                                                         0.00
          MOTA
                  2751 3HG1 VAL B
                                                                                 H
                                       -36.463
-38.228
                                     1
                                                 34.319
                                                          -5.351
                                                                  1.00
                                                                         0.00
          ATOM
                                                                                 H
                  2752 1HG2 VAL B
                                     1
                                                  31.983
55
                                                          -4.860
                                                                  1.00
                                                                         0.00
          ATOM
                  2753 2HG2 VAL B
                                                                                 H
                                     1
                                       -36.576
                                                 31.696
                                                          -4.412
                                                                  1.00
          MOTA
                  2754 3HG2 VAL B
                                                                         0.00
                                     1
                                       -38.001
                                                 31.421
                                                          -3.249
          MOTA
                                                                  1.00
                                                                         0.00
                                                                                 H
                  2755
                       N
                            PRO B
                                    2
                                       -35.933
                                                 32.030
                                                          -0.959
                                                                  1.00
                                                                         0.15
          MOTA
                 2756
                                                                                 N
                        CA
                           PRO B
                                    2
                                       -36.195
                                                 31.541
                                                           0.363
                                                                  1.00
                                                                        0.15
          MOTA
                 2757
                                                                                 C
                        С
                            PRO B
                                    2
                                       -35.493
                                                 32.410
                                                           1.350
60
                                                                  1.00
          ATOM
                                                                        0.15
                 2758
                        0
                            PRO B
                                    2
                                       -34.546
                                                 33.097
                                                           0.973
                                                                  1.00
                                                                        0.15
          ATOM
                                                                                 0
                 2759
                        CB
                            PRO B
                                    2
                                       -35.731
                                                 30.088
                                                           0.391
                                                                  1.00
                                                                        0.15
          ATOM
                 2760
                                                                                 C
                       CG
                            PRO B
                                    2
                                       -35.897
                                                 29.635
                                                         -1.067
                                                                  1.00
                                                                        0.15
          ATOM
                                                                                 С
                 2761
                       CD
                            PRO B
                                       -35.709
                                                 30.924
                                                          -1.884
                                                                  1.00
          MOTA
                                                                        0.15
                                                                                 C
                 2762
                       HA
                            PRO B
                                    2
                                       -37.285
                                                 31.530
65
                                                          0.558
                                                                  1.00
                                                                        0.00
          MOTA
                                                                                 н
                 2763 1HB
                            PRO B
                                    2
                                       -36.304
                                                 29.496
                                                          1.118
                                                                  1.00
                                                                        0.00
          ATOM
                 2764 2HB
                                                                                Н
                            PRO B
                                       -34.669
                                                 30.026
                                                          0.677
                                                                  1.00
          ATOM
                 2765 1HG
                                                                        0.00
                                                                                H
                           PRO B
                                       -36.917
                                                 29.240
                                                         -1.212
                                                                 1.00
                                                                        0.00
         MOTA
                 2766 2HG
                                                                                H
                           PRO B
                                    2
                                       -35.203
                                                 28.833
                                                         -1.366
                                                                 1.00
                                                                        0.00
         ATOM
                 2767 1HD
                                                                                H
                           PRO B
                                    2
                                       -34.667
70
                                                 30.980
                                                         -2.239
                                                                 1.00
                                                                        0.00
         ATOM
                 2768 2HD
                                                                                H
                           PRO B
                                    2
                                       -36.339
                                                         -2.732
                                                 30.824
                                                                 1.00
                                                                        0.00
         MOTA
                                                                                Н
                 2769 N
                                   3 -35.941
                           GLN B
                                                32.393
                                                          2.617
                                                                 1.00
                                                                        0.19
```

5	ATO ATO OTA OTA OTA OTA OTA OTA	M 2771 M 2772 M 2773 M 2774 M 2775	CA GLN C GLN O GLN CB GLN CG GLN CD GLN OE1 GLN	B B B B	3 -35.3 3 -33.5 3 -35.9 3 -35.4 3 -36.3	901 32.7 553 31.6 986 33.0 193 34.0 127 33.8	93 3.76 70 3.3 63 4.9 64 6.0 44 7.29	03 1.00 39 1.00 96 1.00 40 1.00	
10	ATON ATON ATON ATON	M 2777 M 2778 M 2779 M 2780 1	NE2 GLN 1 H GLN 1 HA GLN 1 HB GLN 1	3 3 3	3 -36.9 3 -36.3 3 -36.6 3 -35.4 3 -35.8 3 -37.0	74 34.8 86 31.7 01 34.2 28 32.0	69 8.18 83 2.90 70 3.28 30 5.35	15 1.00 9 1.00 9 1.00 1 1.00	0.19 O 0.19 N 0.00 H 0.00 H
15	ATOM ATOM ATOM ATOM	1 2783 21 1 2784 11 2785 21 2786 1	HG GLNE HG GLNE HE2 GLNE	3 3	3 -35.5 3 -34.4 3 -36.2 3 -37.0	96 35.09 44 33.83 82 35.83 49 34.69	97 5.66 79 6.30 16 7.85 98 8.92	9 1.00 3 1.00 7 1.00 1 1.00	0.00 H 0.00 H 0.00 H 0.00 H
20	ATOM ATOM ATOM ATOM ATOM	2788 0 2789 0 2790 0 2791 0	LYS B LYS B LYS B LYS B LYS B LYS B	4	-31.62 -31.28 -31.66 -30.72	26 33.39 32 32.92 57 33.51 22 34.59	90 4.21 9 5.59 8 6.60 3 3.90	9 1.00 4 1.00 3 1.00 4 1.00	0.23 N 0.23 C 0.23 C 0.23 O 0.23 C
25	ATOM ATOM ATOM ATOM ATOM ATOM	2793 C 2794 N 2795 H 2796 H	LYS B	4 4 4 4	-31.03 -30.32 -33.28 -31.44	36.47 2 37.62 0 38.90 2 34.64 2 32.66	7 2.241 4 2.856 7 2.659 8 4.377	1.00 5 1.00 1.00 1.00	0.23 C 0.23 C 0.23 C 0.23 N1+ 0.00 H
30	ATOM ATOM ATOM ATOM ATOM	2797 1H 2798 2H 2799 1H 2800 2H 2801 1H	B LYS B G LYS B G LYS B D LYS B	4 4 4 4	-29.66 -30.95 -31.91 -30.36 -30.13	2 35.390 9 35.129 0 34.380 2 36.650	3 4.096 8 4.623 9 2.150 0 1.801	1.00 1.00 1.00	0.00 H 0.00 H 0.00 H 0.00 H
35	ATOM ATOM ATOM ATOM	2802 2H 2803 1H 2804 2H 2805 1H 2806 2H	E LYS B E LYS B LYS B LYS B	4 4 4 4	-29.200 -31.168 -32.027 -30.819 -29.420	37.502 7 37.717 9 39.699 38.885	3.942 2.391 3.042	1.00 1.00 1.00	0.00 H 0.00 H 0.00 H 0.00 H 0.00 H
40	ATOM ATOM ATOM ATOM ATOM	2807 3Hz 2808 N 2809 CA 2810 C 2811 O	PRO B PRO B PRO B	4 5 5 5 5	-30.141 -30.550 -30.108 -29.273 -28.730	31.853 31.251 32.279 33.147	1.685 5.616 6.840 7.522	1.00 1.00 1.00 1.00	0.00 H 0.25 N 0.25 C
45	ATOM ATOM ATOM ATOM ATOM	2812 CB 2813 CG 2814 CD 2815 HA 2816 1HB	PRO B	5 5 5 5	-29.231 -28.592 -29.678 -30.972 -29.730	30.082 30.609	6.411 5.112 4.507 7.456 6.357	1.00 (1.00 (1.00 (1.00 (0.25 C 0.25 C 0.25 C 0.00 H
50	ATOM ATOM ATOM ATOM ATOM	2817 2HB 2818 1HG 2819 2HG 2820 1HD 2821 2HD	PRO B PRO B PRO B PRO B	5 5 5 5	-28.453 -28.174 -27.910 -29.236 -30.320	29.911 29.894 31.344 32.397 31.045	7.178 4.412 5.421 4.044	1.00 0 1.00 0 1.00 0	.00 н .00 н .00 н
55	MOTA MOTA MOTA MOTA MOTA	2822 N 2823 CA 2824 C 2825 O 2826 CB	LYS B LYS B LYS B LYS B	6 6 6	-29.172 -28.336 -27.209 -27.391 -29.033	32.227 33.181 32.429 31.333 33.969	3.774 8.861 9.520 10.136 10.666	1.00 0 1.00 0 1.00 0 1.00 0	.00 H .35 N .35 C .35 C
60	ATOM ATOM ATOM ATOM ATOM	2827 CG 2828 CD 2829 CE 2830 NZ 2831 H	LYS B LYS B LYS B LYS B	6 6 6	-30.016 -31.243 -32.218 -33.370	35.023 34.436 35.501 34.856	10.641 10.127 9.427 8.920 8.253	1.00 0. 1.00 0.	.35 C .35 C .35 C .35 C
65	ATOM ATOM ATOM ATOM	2832 HA 2833 1HB 2834 2HB 2835 1HG	LYS B LYS B LYS B	6 - 6 - 6 -	-29.531 -27.947 -28.241 -29.641 -29.498	31.470 33.923 34.472 33.423 35.712	8.805 11.226 11.336	1.00 0. 1.00 0. 1.00 0.	00 H 00 H 00 H 00 H
70	ATOM ATOM ATOM	2836 2HG 2837 1HD 2838 2HD 2839 1HE 2840 2HE	LYS B LYS B	6 - 6 - 6 -	-30.343 -31.763 -30.880 -31.740 -32.610	35.645 33.748 33.844 36.167 36.120	10.981 10.116 8.600 8.183	1.00 0. 1.00 0. 1.00 0. 1.00 0.	00 Н 00 Н 00 Н

193

Н

С

C

Н

H

H

H

H

Н

Н

H

MOTA 2841 1HZ LYS B 6 -33.989 35.514 7.805 1.00 0.00 ATOM 2842 2HZ LYS B 6 -33.032 34.222 7.532 1.00 0.00 MOTA 2843 3HZ LYS B -33.939 34.311 8.889 1.00 0.00 ATOM 2844 N VAL B -25.995 32.999 10.051 1.00 0.35 5 ATOM 2845 CA VAL B 7 -24.871 32.349 10.651 1.00 0.35 ATOM 2846 С VAL B 7 -24.592 33.074 11.922 1.00 0.35 MOTA 2847 7 -24.524 0 VAL B 34.302 11.950 1.00 0.35 ATOM 2848 VAL B CB 7 -23.627 32.383 9.806 1.00 0.35 MOTA 2849 CG1 VAL B -23.210 33.847 9.585 1.00 0.35 10 ATOM 2850 CG2 VAL B 7 -22.552 31.531 10.499 1.00 0.35 ATOM 2851 VAL B Н 7 -25.821 33.888 9.614 1.00 0.00 ATOM 2852 HA VAL B 7 -25.120 31.291 10.831 1.00 0.00 MOTA 2853 HB VAL B 7 -23.863 31.925 8.827 1.00 0.00 MOTA 2854 1HG1 VAL B -22.471 33.901 8.765 1.00 15 0.00 MOTA 2855 2HG1 VAL B 7 -24.031 34.516 9.285 1.00 0.00 ATOM 2856 3HG1 VAL B 7 -22.693 34.280 10.456 1.00 0.00 ATOM 2857 1HG2 VAL B -21.678 31.367 9.847 1.00 0.00 7 ATOM 2858 2HG2 VAL B -22.176 11.412 10.791 32.022 1.00 0.00 ATOM 2859 3HG2 VAL B 7 -22.944 30.551 20 1.00 0.00 MOTA 2860 N SER B 8 -24.448 32.318 13.023 1.00 0.17 ATOM N -24.199 2861 CA SER B 8 32.937 14.287 1.00 0.17 C MOTA 2862 С SER B 8 -22.807 32.592 14.689 1.00 0.17 С MOTA 2863 0 SER B 8 -22.347 31.470 14.481 1.00 0.17 0 MOTA 2864 CB SER B 8 -25.131 32.446 15.407 1.00 0.17 25 С ATOM 2865 OG SER B 8 -24.819 33.105 16.625 1.00 0.17 O MOTA 2866 H SER B 8 -24.625 31.319 13.016 1.00 0.00 н MOTA 2867 HA SER B 8 -24.337 34.028 14.216 1.00 0.00 Н MOTA 2868 1HB SER B 8 -25.073 31.358 15.536 1.00 0.00 ATOM H 2869 2HB SER B 8 -26.174 32.697 15.163 1.00 0.00 30 H P.TOM 2870 HG SER B 8 -24.204 32.543 17.125 1.00 0.00 H MOTA 2871 N LEU B 9 -22.092 33.571 15.268 1.00 0.11 N MOTA 2872 CA LEU B 9 -20.747 33.327 15.682 1.00 0.11 C ATOM 2873 С LEU B 9 -20.696 33.497 17.164 1.00 0.11 С ATOM 2874 0 LEU B 9 -21.139 34.512 17.700 1.00 0.11 35 MOTA 2875 CB LEU B 9 -19.749 34.334 15.080 1.00 0.11 С MOTA 2876 CG LEU B 9 -18.287 34.121 15.512 1.00 0.11 С MOTA 9 -17.732 2877 CD1 LEU B 32.785 14.988 1.00 0.11 С ATOM 2878 CD2 LEU B 9 -17.418 35.324 15.111 1.00 0.11 С ATOM 2879 LEU B H 9 -22.472 34.471 15.510 1.00 0.00 40 Н ATOM 2880 HA T.EII R 9 -20.438 32.317 15.382 1.00 0.00 Н MOTA 2881 1HB LEU B -20.066 35.356 15.354 1.00 0.00 ATOM Н 2882 2HB LEU B 9 -19.814 34.285 13.978 1.00 0.00 Н ATOM 2883 9 -18.324 HG LEU B 33.885 16.546 1.00 0.00 H ATOM 2884 1HD1 LEU B 9 -16.651 32.745 15.192 1.00 0.00 45 Н ATOM 2885 2HD1 LEU B 9 -18.211 31.936 15.488 1.00 0.00 Н MOTA 2886 3HD1 LEU B 9 -17.848 32.744 13.899 1.00 0.00 Н ATOM 2887 1HD2 LEU B 9 -16.368 35.176 15.400 1.00 0.00 ATOM 2888 2HD2 LEU B 9 -17.440 35.449 14.015 1.00 0.00 H ATOM 2889 3HD2 LEU B LEU B 9 -17.775 ASN B 10 -20.176 36.256 15.559 1.00 0.00 Н 50 ATOM 2890 N 32.478 1.00 17.872 0.17 N MOTA 2891 CA ASN B 10 -20.046 32.599 19.291 1.00 0.17 C ATOM 2892 С ASN B 10 -18.653 32.180 19.623 1.00 0.17 С ATOM 10 -18.240 ASN B 2893 0 31.069 19.295 1.00 0.17 0 MOTA 2894 СВ ASN B 10 -20.992 31.672 20.070 1.00 0.17 C 55 MOTA 2895 CG ASN B 10 -22.415 32.145 19.819 1.00 0.17 C ATOM 2896 OD1 ASN B 10 -23.167 31.505 19.086 1.00 0.17 0 MOTA 2897 ND2 ASN B 10 -22.798 33.292 20.443 1.00 0.17 N MOTA 2898 H ASN B 10 -19.879 31.604 17.447 1.00 0.00 H MOTA 2899 HA ASN B 10 -20.331 33.609 19.576 1.00 0.00 60 H ATOM 2900 1HB ASN B 10 -20.745 31.729 21.143 1.00 0.00 Н ATOM 2901 2HB ASN B 10 -20.916 30.627 1.00 19.757 0.00 Н MOTA 2902 1HD2 ASN B 10 -22.191 33.807 21.049 1.00 0.00 H ATOM 2903 2HD2 ASN B 10 -23.731 33.618 20.254 1.00 0.00 Н ATOM 2904 N PRO B 11 -17.897 33.038 20.245 1.00 0.35 65 N MOTA 2905 CA PRO B 11 -18.370 34.356 20.559 1.00 0.35 С MOTA 2906 C PRO B 11 -18.404 35.166 19.305 1.00 0.35 MOTA 2907 0 PRO B 11 -17.867 34.727 18.290 1.00 0.35 0 ATOM 2908 CB PRO B 11 -17.403 34.908 21.604 1.00 0.35 C MOTA 2909 PRO B 11 CG -16.865 33.651 22.308 1.00 0.35 70 ATOM 2910 PRO B CD 11 -16.938 32.559 21.228 1.00 0.35 MOTA 2911 HA PRO B 11 -19.324 34.263 21.103 1.00 0.00

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ATOM
                      2912 1HB
                                PRO B
                                       11
                                           -17.861
                                                      35.651 22.273 1.00 0.00
                                                                                      н
              ATOM
                     2913 2HB
                                PRO B
                                            -16.571
                                        11
                                                      35.402
                                                              21.082
                                                                       1.00
                                                                             0.00
              ATOM
                     2914 1HG
                                                                                      H
                                PRO R
                                        11
                                            -17.522
                                                      33.393
                                                              23.155
                                                                       1.00
                                                                             0.00
              ATOM
                     2915 2HG
                                                                                      Н
                                            -15.851
                                PRO B
                                        11
                                                     33.769
                                                              22.721
     5
                                                                       1.00
              ATOM
                                                                             0.00
                                                                                      H
                     2916
                          1HD
                                PRO B
                                       11
                                            -15.961
                                                     32.431
                                                              20.733
                                                                       1.00
                                                                             0.00
              ATOM
                     2917 2HD
                                                                                      H
                                PRO R
                                        11
                                            -17.234
                                                     31.578
                                                              21.626
                                                                       1.00
             ATOM
                                                                             0.00
                     2918
                                                                                      H
                           N
                                PRO B
                                       12
                                            -19.030
                                                     36.309
                                                              19.364
                                                                       1.00
                                                                             0.52
             ATOM
                     2919
                                                                                      N
                           CA
                                PRO B
                                       12
                                           -19.156
-17.853
                                                     37.156
                                                              18.209
                                                                       1.00
             ATOM
                                                                             0.52
                     2920
                           С
                                                                                      C
                                PRO B
                                       12
                                                     37.765
   10
                                                              17.809
                                                                       1.00
                                                                             0.52
             ATOM
                     2921
                           0
                                PRO B
                                                                                      C
                                       12
                                           -17.789
                                                     38.365
                                                              16.737
                                                                       1.00
                                                                             0.52
             ATOM
                     2922
                                                                                      0
                           CB
                                PRO B
                                       12
                                           -20.215
                                                     38.194
                                                              18.568
                                                                      1.00
                                                                             0.52
             MOTA
                     2923
                                                                                      С
                           CG
                                PRO B
                                           -21.088
                                       12
                                                     37.480
                                                              19.613
                                                                      1.00
             ATOM
                                                                             0.52
                                                                                      C
                     2924
                           CD
                                PRO B
                                       12
                                           -20.128
                                                     36.495
                                                              20.299
             MOTA
                                                                      1.00
                                                                             0.52
                     2925
                                                                                     C
                           HA
                               PRO B
                                       12
                                           -19.493
                                                     36.561
   15
                                                              17.344
                                                                      1.00
                                                                             0.00
             MOTA
                     2926 1HB
                                                                                     H
                               PRO B
                                       12
                                           -20.767
                                                     38.562
                                                              17.689
                                                                      1.00
             ATOM
                                                                             0.00
                     2927 2HB
                                                                                     H
                               PRO B
                                       12
                                           -19.734
                                                     39.074
                                                              19.029
                                                                      1.00
                                                                            0.00
             MOTA
                     2928 1HG
                               PRO B
                                                                                     Н
                                       12
                                           -21.889
                                                     36.926
                                                             19.096
                                                                      1.00
                                                                            0.00
             MOTA
                     2929
                                                                                     H
                          2HG
                               PRO B
                                       12
                                           -21.583
                                                     38.161
                                                             20.323
                                                                      1.00
                                                                            0.00
             MOTA
                     2930 1HD
                                                                                     H
                               PRO B
                                       12
                                           -19.742
                                                     36.914
   20
                                                             21.242
                                                                      1.00
             MOTA
                                                                            0.00
                    2931 2HD
                                                                                     Н
                               PRO B
                                      12
                                           -20.663
                                                    35.567
                                                             20.521
             ATOM
                                                                      1.00
                                                                            0.00
                                                                                     Н
                    2932
                          N
                               TRP B
                                      13
                                           ~16.809
                                                    37.635
                                                             18.646
                                                                      1.00
                                                                            0.35
             MOTA
                                                                                     N
                    2933
                          CA
                               TRP B
                                      13
                                           -15.559
                                                    38.278
                                                             18.359
                                                                      1.00
                                                                            0.35
            MOTA
                    2934
                                                                                     С
                          С
                               TRP B
                                      13
                                           ~15.107
                                                    37.850
                                                             16.998
                                                                      1.00
            ATOM
                    2935
                                                                            0.35
                          0
                               TRP B
                                      13
                                           -14.934
                                                    36.662
  25
                                                             16.731
            MOTA
                                                                      1.00
                                                                            0.35
                                                                                     0
                    2936
                          CB
                               TRP B
                                      13
                                           -14.454
                                                    37.907
                                                             19.361
                                                                      1.00
                                                                            0.35
            ATOM
                                                                                     С
                    2937
                          CG
                               TRP B
                                      13
                                           -14.839
                                                    38.183
                                                             20.795
                                                                      1.00
                                                                            0.35
                                                                                     C
            ATOM
                    2938
                          CD1 TRP B
                                      13
                                           -14.961
                                                    37.307
                                                             21.833
                                                                     1.00
            ATOM
                                                                            0.35
                                                                                     С
                    2939
                          CD2 TRP B
                                      13
                                           -15.219
                                                    39.470
                                                             21.302
                    2940
                                                                     1.00
                                                                            0.35
            ATOM
                                                                                     С
                          NE1 TRP B
                                      13
                                          -15.382
                                                    37.969
  30
                                                             22.961
                                                                     1.00
            ATOM
                                                                            0.35
                                                                                    N
                    2941
                          CE2 TRP B
                                      13
                                          -15.549
                                                    39.302
                                                             22.647
                                                                     1.00
                                                                            0.35
            MOTA
                    2942
                          CE3 TRP B
                                                                                    С
                                      13
                                          -15.297
                                                    40.691
                                                             20.695
                                                                     1.00
            ATOM
                    2943
                                                                            0.35
                                                                                    C
                          CZ2 TRP B
                                      13
                                          -15.962
                                                    40.356
                                                             23.408
                                                                     1.00
                                                                           0.35
            MOTA
                                                                                    C
                    2944
                          CZ3 TRP B
                                      13
                                          -15.707
                                                    41.756
                                                            21.468
                                                                     1.00
                                                                           0.35
            ATOM
                                                                                    С
                   2945
                          CH2
                              TRP B
                                     13
  35
                                          -16.031
                                                    41.590
                                                            22.798
                                                                     1.00
                                                                           0.35
            ATOM
                   2946
                                                                                    С
                          H
                              TRP B
                                     13
                                          -16.882
                                                    37.089
                                                            19.485
                                                                     1.00
                                                                           0.00
            ATOM
                                                                                    H
                   2947
                          HA
                              TRP B
                                          -15.723
                                     13
                                                    39.368
                                                            18.375
                                                                     1.00
                                                                           0.00
            ATOM
                   2948 1HB
                              TRP B
                                                                                    H
                                     13
                                          -13.543
                                                    38.459
                                                            19.077
                                                                     1.00
            MOTA
                                                                           0.00
                                                                                    Н
                   2949 2HB
                              TRP B
                                     13
                                         -14.206
                                                   36.841
                                                            19.251
                                                                     1.00
                                                                           0.00
           ATOM
                   2950
                                                                                    H
                         HD1
                              TRP B
                                     13
                                          -14.738
                                                   36.249
 40
                                                            21.844
                                                                     1.00
                                                                           0.00
           ATOM
                   2951
                                                                                    H
                         HE1
                              TRP B
                                     13
                                          -15.808
                                                   37.524
                                                            23.741
                                                                     1.00
           MOTA
                   2952
                                                                           0.00
                                                                                    H
                         HE3 TRP B
                                          -15.044
                                     13
                                                   40.835
                                                            19.655
                                                                     1.00
                                                                           0.00
           ATOM
                                                                                    Н
                   2953
                         HZ2
                              TRP B
                                     13
                                         -16.229
                                                   40.119
                                                            24.420
           ATOM
                                                                    1.00
                                                                           0.00
                   2954
                                                                                   H
                         HZ3
                             TRP B
                                     13
                                          -15.795
                                                   42.752
                                                            21.062
                                                                    1.00
                                                                           0.00
           ATOM
                   2955
                                                                                   H
                         HH2 TRP B
                                     13
                                         -16.099
                                                   42.501
 45
                                                            23.378
                                                                    1.00
           ATOM
                                                                           0.00
                   2956
                         N
                             ASN B
                                     14
                                         -14.933
                                                   38.829
                                                            16.085
           ATOM
                                                                    1.00
                                                                           0.15
                   2957
                                                                                   N
                         CA
                             ASN B
                                     14
                                         -14.506
                                                   38.539
                                                            14.747
                                                                    1.00
                                                                           0.15
           MOTA
                                                                                   C
                   2958
                         С
                             ASN B
                                     14
                                         -13.076
                                                   38.108
                                                            14.777
                                                                    1.00
                                                                          0.15
           ATOM
                   2959
                                                                                   C
                         0
                             ASN B
                                     14
                                         -12.681
                                                   37.185
                                                            14.064
                                                                    1.00
           ATOM
                  2960
                                                                          0.15
                                                                                   0
                         CB
                             ASN B
                                     14
                                         -14.605
                                                   39.739
                                                           13.785
 50
           MOTA
                                                                    1.00
                                                                          0.15
                  2961
                                                                                   C
                         CG
                             ASN B
                                     14
                                                   40.802
                                         -13.588
                                                           14.181
                                                                    1.00
                                                                          0.15
           ATOM
                                                                                   C
                  2962
                         OD1 ASN B
                                     14
                                         -13.408
                                                   41.115
                                                           15.357
                                                                    1.00
                                                                          0.15
           ATOM
                  2963
                                                                                   ٥
                         ND2 ASN B
                                    14
                                         -12.882
                                                   41.367
                                                           13.165
                                                                    1.00
           ATOM
                                                                          0.15
                  2964
                        H
                             ASN B
                                    14
                                         -15.118
                                                  39.805
                                                           16.295
                                                                    1.00
                                                                          0.00
           MOTA
                                                                                   H
                  2965
                        HA
                             ASN B
                                    14
                                         -15.111
                                                  37.712
 55
                                                           14.342
                                                                    1.00
                                                                          0.00
           ATOM
                  2966
                       1HB
                             ASN B
                                                                                   Н
                                    14
                                         -15.612
                                                  40.188
                                                           13.806
                                                                    1.00
                                                                          0.00
          ATOM
                  2967
                                                                                   H
                       2HB
                             ASN B
                                    14
                                         -14.421
                                                  39.365
                                                           12.763
                                                                    1.00
           ATOM
                                                                          0.00
                                                                                   н
                  2968
                       1HD2 ASN B
                                    14
                                         -12.987
                                                  41.087
                                                           12.202
                                                                   1.00
          MOTA
                                                                          0.00
                  2969
                       2HD2
                                                                                  Н
                            ASN B
                                    14
                                         -12.217
                                                  42.087
                                                           13.380
                                                                   1.00
                                                                          0.00
          MOTA
                  2970
                                                                                  H
                        N
                            ARG B
                                    15
                                        -12.257
                                                  38.773
                                                           15.615
60
                                                                   1.00
          MOTA
                                                                          0.13
                  2971
                                                                                  N
                        CA
                            ARG B
                                    15
                                        -10.859
                                                  38.466
                                                           15.668
                                                                   1.00
                                                                          0.13
          MOTA
                                                                                  C
                  2972
                        С
                            ARG B
                                    15
                                        -10.645
                                                  37.619
                                                           16.872
                                                                   1.00
                                                                          0.13
          ATOM
                  2973
                                                                                  C
                        0
                            ARG R
                                    15
                                        -11.086
                                                  37.958
                                                           17.969
                                                                   1.00
                                                                         0.13
          ATOM
                                                                                  0
                 2974
                        CB
                            ARG B
                                    15
                                         -9.961
                                                  39.702
                                                           15.860
                                                                   1.00
          ATOM
                                                                         0.13
                                                                                  C
                 2975
                        CG
                            ARG B
                                    15
                                         -9.990
                                                  40.695
                                                          14.698
65
                                                                   1.00
                                                                         0.13
          MOTA
                                                                                  C
                 2976
                        CD
                            ARG B
                                    15
                                         -9.087
                                                  41.910
                                                          14.925
                                                                   1.00
                                                                         0.13
          ATOM
                 2977
                                                                                  C
                        NE
                            ARG B
                                    15
                                         -9.233
                                                  42.805
                                                          13.742
                                                                   1.00
          MOTA
                                                                         0.13
                 2978
                        CZ
                            ARG B
                                    15
                                         -8.137
                                                  43.184
                                                          13.023
                                                                   1.00
                                                                         0.13
          ATOM
                                                                                  C
                 2979
                       NH1
                            ARG B
                                   15
                                         -6.892
                                                  42.769
                                                          13.396
                                                                   1.00
          ATOM
                                                                         0.13
                 2980
                                                                                  N
                       NH2
                           ARG B
                                   15
                                         -8.289
                                                 43.984
70
                                                          11.926
                                                                   1.00
                                                                         0.13
          MOTA
                                                                                  N
                 2981
                       Н
                            ARG R
                                   15
                                        -12.591
                                                 39.606
                                                          16.079
         MOTA
                                                                   1.00
                                                                         0.00
                 2982
                                                                                  Н
                       HA
                           ARG B
                                        -10.563
                                                 37.963
                                                          14.736
                                                                  1.00
                                                                         0.00
```

	ATO	4 2983 1	HB ARG	B 15	-8.99	6 39.35	0 16.21	4 1.00	0.00	
	ATO			B 15	-10.35	4 40.25				
	ATOR AOTA								0.00	
5	ATOM									
	ATOM	1 2988 21	ID ARG							
	ATOM		IE ARG	B 15	–	1 43.52				
	ATOM ATOM	f 2990 1F	H1 ARG	B 15	–					н
10	ATOM		H2 ARG							H
	ATOM		H2 ARG	B 15						H
	ATOM	2994 N								H
	ATOM		A ILE							N C
15	MOTA MOTA	_			-8.300			1.00		č
	ATOM		B ILE		-7.583 -10.558					0
	MOTA		G1 ILE		-10.336				0.12 0.12	c
	ATOM		G2 ILE	B 16	-12.035	34.818			0.12	C C
20	MOTA		D1 ILE		-10.816		16.840		0.12	č
2.0	MOTA MOTA				-9.589				0.00	H
	ATOM				-9.806 -10.323				0.00	H
	ATOM	3005 1H	G1 ILE	B 16	-9.151				0.00	H
25	ATOM	3006 2H	31 ILE	B 16	-10.632				0.00	H H
25	ATOM ATOM	3007 1H	32 ILE 1	B 16	-12.707	33.959	18.128		0.00	H
	ATOM	3008 2H 3009 3H	32 ILE 1 22 TTE 1		-12.205				0.00	H
	ATOM	3010 1H	Ol ILE	B 16 B 16	-12.376 -10.934				0.00	H
20	MOTA	3011 2H	1 ILE	3 16	-10.156		15.860 17.441	1.00 1.00	0.00 0.00	H
30	ATOM		1 ILE P		-11.792		17.336	1.00	0.00	H H
	ATOM ATOM	3013 N 3014 C	PHE I		-7.862	34.506	18.848	1.00	0.17	N
	ATOM	3014 C	PHE E		-6.527 -6.595	33.996 32.557	18.904	1.00	0.17	С
	ATOM	3016 0	PHE E		-7.645	31.923	18.543 18.627	1.00	0.17	C
35	MOTA	3017 CE	PHE E		-5.886	33.999	20.300	1.00 1.00	0.17 0.17	O C
	MOTA	3018 CG			-5.562	35.386	20.720	1.00	0.17	č
	ATOM ATOM		1 PHE B		-4.468	36.028	20.192	1.00	0.17	С
	ATOM		1 PHE B		-6.337 -4.154	36.026	21.657	1.00	0.17	С
4 0	MOTA		2 PHE B		-6.027	37.305 37.303	20.585	1.00 1.00	0.17 0.17	C
	ATOM	3023 CZ			-4.935	37.939	21.518	1.00	0.17	C C
	ATOM ATOM	3024 H	PHE B		-8.467	34.178	19.583	1.00	0.00	н
	ATOM	3025 HA 3026 1HB	PHE B	17 17	-5.913	34.589	18.229	1.00	0.00	H
45	ATOM	3027 2HB	PHE B	17	-4.946 -6.495	33.448 33.466	20.184 21.041	1.00	0.00	H
	ATOM		1 PHE B	17	-3.883	35.515	19.440	1.00 1.00	0.00	H H
	ATOM		PHE B	17	-7.205	35.518	22.059	1.00	0.00	H
	ATOM ATOM		l PHE B	17	-3.236	37.726	20.300	1.00	0.00	H
50	ATOM	3032 HZ	PHE B	17 17	-6.677 -4.353	37.770	22.777	1.00	0.00	H
	ATOM	3033 N	LYS B	18	-5.446	38.631 32.008	22.047 18.119	1.00 1.00	0.00	H
	ATOM	3034 CA	LYS B	18	~5.403	30.623	17.781	1.00	0.22 0.22	N C
	ATOM	3035 C	LYS B	18	-5.558	29.867	19.056	1.00	0.22	č
55	ATOM ATOM	3036 O 3037 CB	LYS B LYS B	18	-5.134	30.320	20.119	1.00	0.22	0
	ATOM	3038 CG	LYS B	18 18	-4.077 -2.859	30.203 30.461	17.126	1.00	0.22	С
	ATOM	3039 CD	LYS B	18	-1.586	29.780	18.012 17.511		0.22	C
	ATOM	3040 CE	LYS B	18	-0.375	29.996	18.418		0.22 0.22	C C
60	ATOM	3041 NZ	LYS B	18	0.743	29.138	17.967		0.22	N1+
00	ATOM ATOM	3042 н 3043 на	LYS B	18	-4.641	32.589	17.925	1.00	0.00	H
	ATOM	3044 1HB	LYS B LYS B	18 18	-6.267 -3.964	30.489	17.128		0.00	H
	ATOM	3045 2HB	LYS B	18	-4.150	30.718 29.124	16.156 16.902		0.00	H
65	ATOM	3046 1HG	LYS B	18	-3.038	30.058	19.019		0.00 0.00	H H
0 3	MOTA	3047 2HG	LYS B	18	-2.689	31.546	18.128		0.00	H
	ATOM ATOM	3048 1HD 3049 2HD	LYS B	18		30.137	16.492	1.00	0.00	H
	ATOM	3050 1HE	LYS B LYS B	18 18		28.698		1.00	0.00	H
	ATOM	3051 2HE	LYS B			29.719 31.038			0.00	H
70	ATOM	3052 1HZ	LYS B	18).00).00	H H
	ATOM	3053 2HZ	LYS B	18					0.00	H

	ATOM ATOM ATOM	3055	3HZ N CA	LYS GLY GLY	B 1	18 19 19	1.01 -6.20 -6.38	7 28.69	2 18.97	8 1.0	0 0.21	H N
5	ATOM ATOM ATOM ATOM	3057 3058 3059	О Н	GLY GLY	B 1 B 1 B 1	19 19 19	-7.70 -8.19 -6.49	8 28.21 2 27.50 5 28.32	4 20.74 1 21.62 7 18.07	6 1.0 3 1.0 1 1.0	0 0.21 0 0.21	С О Н
10	ATOM ATOM ATOM	3061 3062 3063	2HA N CA	GTA GTA GTA	B 1 B 2 B 2	19 19 10	-5.676 -6.086 -8.336 -9.616	26.83 29.30	8 20.09 6 20.28	6 1.00 1 1.00	0.00	H N C
1.5	MOTA MOTA MOTA MOTA	3065 3066 3067	C O CB CG	GTA GTA GTA	B 2 B 2	0 0 0	-10.642 -10.428 -10.002 -9.106	28.23 2 31.13	1 19.120 0 20.57	2 1.00 3 1.00 4 1.00	0.23 0.23 0.23	0000
15	MOTA MOTA MOTA MOTA	3069		GLU GLU GLU	B 2	0	-9.228 -10.378 -8.174 -7.903	31.77 31.53 31.73	22.806 23.263 23.495	1.00 1.00 1.00	0.23 0.23 0.23	c o o1-
20	MOTA MOTA MOTA	3072 3073 3074 3075	HA 1HB 2HB	GLU GLU	B 2 B 2 B 2	0 0 0	-9.596 -11.054 -9.998	29.463 31.273 31.319	21.915 20.883 19.493	1.00 1.00 1.00	0.00 0.00 0.00	н н н н
25	ATOM ATOM ATOM	3076 : 3077 3078	2HG N CA	GLU : GLU : ASN : ASN :	B 20 B 20 B 20	0 1 1	-9.443 -8.053 -11.794 -12.833	32.040 28.642 27.815	21.031	1.00 1.00	0.00	H H N C
	ATOM ATOM ATOM ATOM	3079 3080 3081 3082	C O CB CG	ASN I ASN I ASN I	B 21	1 1	-13.814 -14.134 -13.589 -12.613	29.792	19.677 20.179 21.415	1.00	0.16 0.16 0.16 0.16	с 0 с
30	MOTA MOTA MOTA MOTA	3083 3084 3085 3086		ASN I ASN I ASN I	3 21 3 21 3 21	l L	-11.595 -12.923 -12.005 -12.376	25.692 25.418 29.178	21.347 23.168 21.704	1.00 1.00 1.00	0.16 0.16 0.00	С 0 N Н
35	ATOM ATOM ATOM ATOM	3087 1 3088 2 3089 1 3090 2	HB HB HD2	ASN E ASN E ASN E	3 21 3 21 3 21		-14.424 -13.999 -13.739	27.142 26.471 27.666 25.683	19.624 20.932 22.196 23.687	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H H
40	MOTA MOTA MOTA	3091 3092 3093	N CA C	VAL B VAL B	22 22 22		-12.261 -14.289 -15.243 -16.438	24.760 28.299 29.093 28.234	23.540 18.490 17.780 17.559	1.00 1.00 1.00	0.00 0.07 0.07 0.07	H C C
	ATOM ATOM ATOM ATOM	3095 3096	CB CG1	VAL B VAL B VAL B VAL B	22	-	-16.312 -14.753 -15.891 -13.481	27.053 29.535 30.274 30.379	17.236 16.431 15.710 16.626	1.00 1.00 1.00 1.00	0.07 0.07 0.07 0.07	0 0 0
45	MOTA MOTA MOTA MOTA	3099	HA '	VAL B VAL B VAL B	22 22 22 22	-	14.083 15.511 14.492 15.529	27.370 29.985 28.689	18.135 18.368 15.799	1.00 1.00 1.00	0.00 0.00 0.00	H H H
50	ATOM ATOM ATOM	3102 21 3103 31 3104 11	HG1 V HG1 V HG2 V	VAL B VAL B VAL B	22 22 22	-	16.697 16.314 13.124	30.772 29.591 31.040 30.786	14.795 15.399 16.376 15.667	1.00 1.00 1.00	0.00 0.00 0.00	H H H H
55	MOTA MOTA MOTA		iG2 \ I 1	VAL B VAL B THR B	22 22 23 23	-	13.699 12.657 17.641 18.823	31.230 29.793 28.800 28.028	17.292 17.064 17.762 17.530	1.00 1.00 1.00 1.00	0.00 0.00 0.06 0.06	H H N C
	ATOM ATOM ATOM ATOM	3111 0) 1 B 1	THR B THR B THR B	23 23 23 23	_	19.615 19.909 19.704 18.992	28.740 29.927 27.891	16.486 16.612 18.737	1.00 1.00 1.00	0.06 0.06 0.06	с 0 с
60	ATOM ATOM ATOM ATOM	3113 C 3114 H 3115 H	G2 I A I	HR B HR B	23 23 23	-: -: -:	20.936 17.770 18.554	27.254 27.053 29.719 27.016	19.787 18.353 18.174 17.215	1.00 1.00 1.00 1.00	0.06 0.06 0.00 0.00	о С Н
65	MOTA MOTA MOTA	3117 H 3118 1H 3119 2H	G1 T G2 T G2 T	HR B	23 23 23 23	-: -:2	20.030 19.557 21.569 21.569	28.886 27.282 26.856 27.557	19.078 20.569 19.233 17.607	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н
70	ATOM ATOM ATOM ATOM ATOM	3120 3H 3121 N 3122 C 3123 C 3124 O	A L L	HR B EU B EU B EU B	23 24 24 24 24	-2 -1 -2 -2	20.629 19.967 20.752 22.058	26.075 28.020 28.613 27.900 26.671	17.945 15.407 14.368 14.393 14.388	1.00 1.00 1.00 1.00	0.00 0.06 0.06 0.06 0.06	H N C C

	ATO	1 3126	CB LEU	B 24					0.06 C
5	ATON ATON	3128 3129	CD1 LEU CD2 LEU H LEU	B 24	4 -18.8	46 28.82° 14 30.541	7 11.352 8 13.167	1.00	0.06 C
	ATOM ATOM ATOM	3131 1 3132 2	HB LEU	B 24	-20.87	58 29.681 76 28.841	14.551 7 12.246	1.00	0.00 H 0.00 H
10	ATOM ATOM ATOM	3134 1 3135 2	HG LEU 1 HD1 LEU 1 HD1 LEU 1	B 24	-17.23	71 28.564 31 29.242	13.461 11.246	1.00 1.00	0.00 H 0.00 H
1.5	MOTA MOTA MOTA	3137 1: 3138 2:	HD1 LEU 1 HD2 LEU 1 HD2 LEU 1	3 24 3 24	-18.89 -17.82	3 29.306 0 30.978	10.600 12.972	1.00 1.00	0.00 H 0.00 H
15	MOTA MOTA MOTA	3139 31 3140 1	HD2 LEU H V THR H LA THR H	3 24 3 25	-19.05 -23.16	8 30.667 7 28.659	14.225 14.441	1.00	0.00 H 0.00 H 0.28 N
20	ATOM ATOM ATOM			25 25		0 28.557 0 29.760	13.308 13.059	1.00 (0.28 C 0.28 C
	ATOM ATOM ATOM	3145 0 3146 0 3147 F	G1 THR B	25 25	-24.523 -26.586 -23.126	3 27.828 0 27.539	15.697 16.841 15.588	1.00 (0.28 C 0.28 O 0.28 C
25	MOTA MOTA MOTA	3149 H	A THR B B THR B G1 THR B	25 25	-24.321 -25.448 -23.678	26.920 29.352	14.385 14.354 15.810 16.823	1.00 0	0.00 н 0.00 н
20	ATOM ATOM ATOM	3151 1H 3152 2H	G2 THR B G2 THR B G2 THR B	25 25 25	-27.114 -27.247 -26.441	27.581	16.552 14.837 15.342	1.00 0 1.00 0	.00 H
30	ATOM ATOM ATOM	3154 N 3155 C 3156 C	CYS B	26 26 26	-25.878 -26.616 -28.050	27.669 28.143	12.565 11.446 11.751	1.00 0 1.00 0	.00 H .52 N .52 C
35	ATOM ATOM ATOM	3157 O 3158 C 3159 S	CYS B	26 26 26	-28.460 -26.230 -27.098	26.734 27.356	11.908 10.198 8.709	1.00 0 1.00 0	.52 C .52 O
	ATOM ATOM ATOM	3160 H 3161 H 3162 1H	CYS B	26 26 26	-25.872 -26.399 -26.355	26.670	12.726 11.235 10.346	1.00 0 1.00 0	.52 S .00 н
40	ATOM ATOM ATOM	3163 2HI 3164 N 3165 C	ASN B	26 27 27	-25.174 -28.853 -30.232	27.547 28.959 28.793	10.007 11.836 12.176	1.00 0. 1.00 0.	.00 H .00 H .35 N
45	ATOM ATOM ATOM	3166 C 3167 O 3168 CE		27 27 27	-31.043 -30.620 -30.713	29.100 29.856 29.749	10.964 10.092 13.280	1.00 0. 1.00 0.	35 C 35 C 35 O 35 C
40	ATOM ATOM ATOM	3171 ND	1 ASN B 2 ASN B	27 27 27	-30.594 -29.551 -31.698	31.169 31.568 31.954	12.743 12.228	1.00 0.	35 C 35 O
50	ATOM ATOM ATOM ATOM	3172 H 3173 HA 3174 1HB	ASN B	27 27	-28.543 -30.415 -30.081	29.920 27.767 29.665	11.683 12.532	1.00 0. 1.00 0. 1.00 0.	00 н 00 н
	ATOM ATOM ATOM	3175 2HB 3176 1HD 3177 2HD	ASN B	27 27	-31.746 -32.530 -31.598		13.557 13.316	1.00 0.0 1.00 0.0 1.00 0.0	00 H
55	ATOM ATOM ATOM	3178 N 3179 CA 3180 C	GLY B GLY B	28 28	-32.237 -33.101 -33.969	28.485 28.725 27.521	10.876 9.762	1.00 0.1 1.00 0.1	15 N 15 C
60	MOTA MOTA	3181 O 3182 H 3183 1HA		28 - 28 -	-33.839 -32.528 -32.514		10.382 1 11.502 1	1.00 0.1 1.00 0.0	15 O 10 H
	ATOM ATOM ATOM ATOM	3184 2HA 3185 N 3186 CA	ASN B ASN B	29 - 29 -	-33.710 -34.882 -35.730	29.632 27.537 26.399	9.918 1 8.633 1	.00 0.0 .00 0.1	00 H .6 N
65	MOTA MOTA	3187 C 3188 O 3189 CB	ASN B	29 - 29 -	-34.852 -33.866 -36.820	25.276 25.478 26.580	8.021 1 7.315 1	.00 0.1 .00 0.1 .00 0.1	6 C
	ATOM ATOM	3192 ND2	ASN B	29 - 29 -	37.878 38.816	27.535 27.893 27.949	7.919 1 9.096 1	.00 0.1 .00 0.1	6 C
70	ATOM	3193 H 3194 HA 3195 1HB	ASN B 2	29 -	36.207		8.013 1 9.419 1	.00 0.00	0 н 0 н

5	ATON ATON ATON ATON ATON ATON	f 3197 f 3198 f 3199 f 3200 f 3201 f 3202	1HD2 2HD2 N CA C	ASN ASN ASN ASN ASN ASN ASN	B 2 B 2 B 3 B 3 B 3 B 3	9 -38.83 9 -39.53 0 -35.18 0 -34.33 0 -35.26 0 -36.42	33 27.63 32 28.56 37 24.05 77 22.92 58 21.82	1 6.076 2 7.386 1 8.463 1 8.123 3 7.645	8 1.00 0 1.00 3 1.00 7 1.00 5 1.00		H H N C C
10	ATOM ATOM ATOM ATOM ATOM ATOM	3204 3205 3206 3207		ASN ASN ASN ASN	B 30 B 30 B 30 B 30	0 -32.79 0 -32.21 0 -32.78 0 -36.00	25 21.178 0 21.159 1 20.126 14 23.852	9.339 8.886 7.805 9.746 9.015	1.00 1.00 1.00 1.00	0.16 0.16 0.16 0.16 0.00	C C N H
15	MOTA MOTA MOTA MOTA MOTA	3209 3210 3211 3212	1HB 2HB 1HD2	ASN I ASN I ASN I ASN I PHE I	B 30 B 30 B 30	-34.30 -32.90 -33.32 -32.19	7 22.117 4 23.133 3 20.099 5 19.340	10.152 9.720 10.587 9.478	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
20	MOTA MOTA MOTA MOTA	3214 3215 3216 3217 3218	CA C O CB CG	PHE I PHE I PHE I PHE I	3 31 3 31 3 31 3 31	-35.48 -35.22 -34.24 -35.02	6 19.863 8 18.765 3 18.805 4 19.385		1.00	0.12 0.12 0.12 0.12 0.12 0.12	и с с с
25	MOTA MOTA MOTA MOTA MOTA	3219 3220 3221 3222 3223	CD2 CE1 CE2 CZ	PHE E PHE B PHE B	31 31 31 31 31	-37.13' -35.39! -37.919 -36.173	7 18.422 5 16.940 9 17.353 8 15.867 9 16.073	3.958 4.581 3.589 4.215 3.720	1.00 1.00 1.00 1.00 1.00	0.12 0.12 0.12 0.12 0.12	00000
30	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3224 3225 3226 3227 3228 3228 3229	HA LHB PHB HD1	PHE B PHE B PHE B PHE B PHE B	31 31 31 31	-33.732 -36.560 -33.955 -35.127 -37.521	20.108 19.120 20.202 19.428	6.678 6.225 4.883 4.121 3.830	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H H
35	MOTA ATOM ATOM ATOM ATOM ATOM	3230 3231 3232 3233 3234	HE1 HE2 HZ	PHE B PHE B PHE B PHE B PHE B	31 31 31 31 32 32	-34.399 -38.916 -35.783 -38.053 -36.111	17.520 14.857 15.224 17.753	4.975 3.188 4.316 3.428 7.268	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00 0.11	H H H N
40	ATOM ATOM ATOM ATOM ATOM	3235 3236 3237 3238	C 1 O 1 CB 1 CG 1	PHE B PHE B PHE B PHE B PHE B	32 32 32 32 32 32	-35.851 -34.911 -35.322 -37.114 -37.971 -38.800	15.762 14.780 15.971 16.991	8.229 7.598 6.982 8.670 9.336	1.00 1.00 1.00 1.00	0.11 0.11 0.11 0.11	C C O C C
45	ATOM ATOM ATOM ATOM ATOM	3240 3241 3242 3243	CD2 F CE1 F CE2 F	PHE B	32 32 32 32 32 32	-36.800 -37.941 -39.597 -38.735 -39.564 -36.832	17.790 17.160 18.739 18.108 18.899	8.583 10.700 9.178 11.300 10.542	1.00 1.00	0.11 0.11 0.11 0.11	0 0 0 0
50	ATOM ATOM ATOM ATOM ATOM	3245 1 3246 11 3247 21 3248 1	IA P	HE B HE B HE B	32 32 32 32 32 32	-35.409 -36.811 -37.630 -38.864 -37.287	17.591 17.166 15.166 15.498 17.652 16.539	6.586 9.143 9.358 7.820 7.507	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H H
55	ATOM ATOM ATOM ATOM ATOM	3250 H 3251 H 3252 H 3253 N	IE1 P IE2 P IZ P I G:	HE B	32 32 32 33 33	-40.252 -38.706 -40.190 -33.600 -32.616	19.360 18.233 19.649 16.034 15.164	11.307 8.572 12.380 11.019 7.738	1.00 (1.00 (1.00 (0.00 0.00 0.00 0.00 0.10	H H H N
60	ATOM ATOM ATOM ATOM ATOM	3255 C 3256 C 3257 C	G G B G G G	LU B LU B LU B LU B	33 33 33	-31.455 -31.273 -32.084 -31.401	15.127 16.029 15.638 17.006	5.809 5.863	1.00 0 1.00 0 1.00 0	0.10 0.10 0.10 0.10	0000
65	ATOM ATOM ATOM ATOM ATOM	3260 O	E1 GI E2 GI GI A GI	UB UB UB	33 33 33 33	-30.934 -30.393 -31.113 -33.258 -33.037	17.340 16.424 18.515 16.896 14.148	3.782 4.035 8.139 7.082	1.00 0 1.00 0 1.00 0 1.00 0	.10 .10 .10 .00	С О О1- Н
70	ATOM ATOM	3265 2H 3266 1H	B GL	UB UB UB	33	-32.872 -31.344 -30.551	15.591 14.879 16.931	5.494	1.00 0	.00 .00 .00	H H H

5	ATON ATON ATON ATON ATON ATON	3268 3269 3270 3271 3272	HG GLU N VAL CA VAL C VAL O VAL CB VAL CGI VAL	B 34 B 34 B 34 B 34 B 34	-30.64 -29.51 -28.55 -28.07 -28.79	4 14.058 1 13.941 9 15.048 7 15.734 2 12.637	8.020 8.884 8.570 9.470 8.712	1.00 1.00 1.00 1.00 1.00	0.00 0.09 0.09 0.09 0.09	H N C C O C
10	ATOM ATOM ATOM ATOM ATOM	3275 1 3276 1 3277 1 3278 1	CG2 VAL 1 H VAL 1 HA VAL 1 HB VAL 1 HG1 VAL 1	B 34 B 34 B 34 B 34	-29.79 -30.815 -29.835 -28.403	7 11.497 5 13.314 5 14.056 3 12.546	8.948	1.00 1.00 1.00 1.00	0.09 0.09 0.00 0.00	C H H H
15	ATOM ATOM ATOM ATOM	3280 31 3281 11 3282 21	HG1 VAL H HG1 VAL H HG2 VAL H HG2 VAL H HG2 VAL H	3 34 3 34 3 34	-26.840 -27.914 -29.295	13.370 12.776 10.514 11.600	9.421 10.716 8.942 9.931 8.178	1.00 1.00	0.00 0.00 0.00 0.00	H H H H
20	ATOM ATOM ATOM ATOM ATOM	3284 N 3285 C 3286 C 3287 C	SER E A SER E SER E	35 35 35 35 35	-28.277 -27.364 -28.183 -28.493 -26.512	15.279 16.335 17.559 17.913	7.274 6.942 6.696 5.559	1.00 1.00 1.00 1.00	0.00 0.11 0.11 0.11	H C C
25	MOTA MOTA MOTA MOTA MOTA		G SER B SER B A SER B B SER B	35 35	-27.339 -28.722 -26.655 -25.922 -25.813	15.843 14.814 16.496 15.124	5.689 4.552 6.501 7.772 5.827	1.00 1.00 1.00 1.00	0.11 0.11 0.00 0.00 0.00	С О Н Н
30	MOTA MOTA MOTA MOTA MOTA	3294 H 3295 N 3296 C 3297 C 3298 O	G SER B SER B	35 36 36 36 36	-27.978 -28.548 -29.398 -28.707	16.882 16.589 18.243 19.394 20.528	5.528 4.533 7.794 7.742 7.057	1.00 1.00 1.00 1.00	0.00 0.00 0.27 0.27 0.27	H H N C
35	ATOM ATOM ATOM ATOM ATOM	3299 C 3300 O 3301 H 3302 HJ 3303 1HJ	SER B SER B SER B SER B	36 36 36 36	-29.282 -29.776 -30.410 -28.475 -30.315	21.190 19.889 18.846 17.775 19.170	6.194 9.147 9.871 8.692 7.176	1.00	0.27 0.27 0.27 0.00 0.00	О С Н Н
40	ATOM ATOM ATOM ATOM ATOM	3304 2HI 3305 HO 3306 N 3307 CA	SER B SER B THR B THR B	36 36 37 37	-30.346 -28.841 -30.330 -27.431 -26.842	20.826 20.156 19.061 20.777 21.964	9.116 9.675 10.811 7.399 6.858	1.00 1.00 1.00	0.00 0.00 0.00 0.48 0.48	H H H N C
45	ATOM ATOM ATOM ATOM	3312 CG	1 THR B 2 THR B	37 37 37 37 37	-25.567 -24.911 -26.522 -25.965 -25.515	21.675 20.660 22.984 24.129 22.381	6.148 6.377 7.901 7.283 8.896	1.00 1.00 1.00	0.48 0.48 0.48 0.48 0.48	0000
50	ATOM ATOM ATOM ATOM ATOM	3317 1HG	THR B 1 THR B 2 THR B	37 37 37 37 37	-26.848 -27.514 -27.418 -25.716 -25.307	20.135 22.445 23.228 24.744 23.154	7.907 6.132 8.460 7.987 9.649	1.00 (1.00 (1.00 (0.00 0.00 0.00 0.00	H H H H
55	ATOM ATOM ATOM ATOM ATOM	3318 2HG 3319 3HG 3320 N 3321 CA 3322 C	2 THR B LYS B	38 38	-25.923 -24.557 -25.205 -23.972 -23.171	21.495 22.126 22.598 22.506 23.683	9.398 8.418 5.235 4.517	1.00 0 1.00 0 1.00 0 1.00 0	.00 .00 .41 .41	H H N C
60	ATOM ATOM ATOM ATOM ATOM	3323 O 3324 CB 3325 CG 3326 CD 3327 CE	LYS B LYS B LYS B LYS B	38 38 38	-26.617	24.798 22.656 21.731 22.138 21.373	5.054 2.995 2.385 2.751	1.00 0 1.00 0 1.00 0 1.00 0	.41 .41 .41	0 C C
65	ATOM ATOM ATOM ATOM ATOM	3328 NZ 3329 H 3330 HA 3331 1HB 3332 2HB	LYS B LYS B LYS B	38 38 38 38	-29.037 -25.630 -23.477 -23.141	21.900 23.518 21.547 22.476 23.693	2.348 5.314 4.738 2.541	1.00 0 1.00 0 1.00 0	.41 .41 .00 .00	C N1+ H H
70	ATOM ATOM ATOM ATOM ATOM	3333 1HG 3334 2HG 3335 1HD 3336 2HD 3337 1HE	LYS B LYS B LYS B	38 - 38 - 38 -	-24.996 -25.082 -26.726 -26.849	20.683 21.760 23.208 21.891	2.681 1 1.285 1 2.649 1 3.795 1	1.00 0. 1.00 0. 1.00 0.	.00 .00 .00	H H H H H

	ATOM	3339		LYS LYS	B 38	-29.78	32 21.422				
	ATOM ATOM		2HZ 3HZ	LYS			27 21.774	3.33			
5	ATOM			LYS TRP							H
	ATOM			TRP							N
	ATOM			TRP	B 39	-20.04					C
	ATOM ATOM			TRP				4.03			ŏ
10	ATOM			TRP TRP							С
	ATOM			TRP						0.18	c
	ATOM	3349		TRP						0.18 0.18	C
	ATOM	3350		TRP						0.18	N
15	MOTA MOTA	3351 3352		TRP					1.00	0.18	Ċ
	ATOM	3353		TRP						0.18	C
	ATOM	3354		TRP						0.18 0.18	C C
	ATOM	3355		TRP I	_					0.18	C
20	ATOM ATOM	3356 3357	H	TRP I		-21.42		5.234		0.00	H
20	ATOM	3358	HA 1HB	TRP I		-21.686 -19.54		5.806		0.00	H
	ATOM	3359	2HB	TRP E		-19.802		7.108 7.047		0.00	H
	ATOM	3360		TRP E	39	-21.773		8.874		0.00	H H
25	ATOM	3361		TRP F		-23.076	23.572	10.695		0.00	H
25	ATOM ATOM	33 62 33 63		TRP E		-20.762		7.571		0.00	H
	ATOM	3364		TRP E		-23.620 -21.828		11.520		0.00	H
	ATOM	3365		TRP B		-23.235		8.842 10.806	1.00 1.00	0.00	H
30	ATOM	3366	N	PHE B		-19.690		4.416	1.00	0.08	H N
30	MOTA MOTA	3367	CA	PHE B		-18.688		3.434	1.00	0.08	Ĉ
	ATOM	3368 3369	С 0	PHE B	40 40	-17.664		4.057	1.00	0.08	С
	ATOM	3370	CB	PHE B	40	-17.990 -19.229		4.811	1.00	0.08	0
2.5	ATOM	3371	CG	PHE B	40	-20.153		2.190 1.514	1.00 1.00	0.08 0.08	C C
35	ATOM	3372		PHE B	40	-21.465	25.994	1.916	1.00	0.08	C
	ATOM ATOM	3373 3374		PHE B	40	-19.703		0.478	1.00	0.08	č
	ATOM	3375		PHE B PHE B	40 40	-22.315 -20.551		1.291	1.00	0.08	С
	ATOM	3376		PHE B	40	-21.860		-0.150 0.257	1.00 1.00	0.08	C
40	ATOM	3377		PHE B	40	-20.105	26.853	4.892	1.00	0.08	C H
	ATOM ATOM	3378		PHE B	40	-18.309	25.372	3.136	1.00	0.00	н
	ATOM			PHE B	40 40	-18.376 -19.730	27.311	1.549	1.00	0.00	H
	ATOM	3381		PHE B	40	-21.845	27.984 26.623	2.471 2.717	1.00 1.00	0.00	H
45	ATOM	3382		PHE B	40	-18.680	25.415	0.131	1.00	0.00	H H
	ATOM	3383		PHE B	40	-23.355	25.087	1.589	1.00	0.00	H
	atom atom	3384 3385	HE2	PHE B	40 40	-20.212	23.880	-1.022	1.00	0.00	H
	ATOM	3386		HIS B	41	-22.535 -16.383	23.650 26.921	-0.252 3.777	1.00	0.00	H
50	MOTA	3387	CA F	HIS B	41	-15.322	27.757	4.242	1.00 1.00	0.10 0.10	N C
	ATOM	3388		HIS B	41	-14.620	28.223	3.014	1.00	0.10	c
	ATOM ATOM	3389 3390		HIS B	41	-14.100	27.419	2.242		0.10	0
	ATOM	3391		IIS B	41 41	-14.287 -13.274	27.030 27.973	5.109		0.10	C
55	ATOM	3392	ND1 E		41	-12.236	27.588	5.682 6.499		0.10 0.10	C N
	ATOM		CD2 H		41	-13.159	29.322	5.541		0.10	C
	ATOM ATOM	3394	CE1 H	IS B	41	-11.548	28.715	6.810		0.10	Č
	ATOM		NE2 H	IS B	41 41	-12.071	29.794	6.253		0.10	N
60	ATOM			IS B	41	-16.137 -15.740	26.064 28.586	3.279 4.831		0.00	H
	MOTA	3398 1	нв н	IS B		-13.799	26.218	4.545		0.00 0.00	H H
	ATOM	3399 2		IS B	41	-14.824	26.533	5.938		0.00	H
	ATOM ATOM		HD2 H			-13.745	30.040	5.019	1.00	0.00	н
65	ATOM		HE1 H HE2 H			-10.615 -11.766	28.670	7.349		0.00	H
	MOTA			SN B		-11.766	30.724 29.547	6.456 2.797		0.00	H
	ATOM	3404	CA A	SN B		-13.967	30.065	1.622).11).11	N C
	ATOM			SN B		-14.617	29.423	0.440		0.11	c
70	ATOM ATOM			SN B SN B		-14.003		-0.614	1.00 0	.11	0
. 🗸	ATOM			on B		-12.450 -11.781	29.807			.11	C
						/01	30.743	2.558	1.00 0	.11	С

	ATON ATON	1 34		D1 ASN D2 ASN ASN	B	42 42 42	-10.44	7 30.56	2.75	8 1.0	0.11	N
5	ATON	1 34	12 H	A ASN	B	42	-14.18	6 31.14	1.52			H H
J	ACTA ACTA	34	13 1H 14 2H	B ASN	В	42						H H
	ATOM ATOM		15 1H 16 2H	D2 ASN D2 ASN	В	42 42	-9.94	1 29.816	2.32	8 1.00	0.00	H
10	ATOM	34	17 N	GLY	В	43	-15.89					H N
10	ATOM ATOM			A GLY GLY		43 43			-0.51	5 1.00	0.08	С
	ATOM ATOM			GLY	В	43	-16.83	0 26.369	-1.54	6 1.00		C O
1 5	ATOM	342	22 1H			43 43						H H
15	ATOM ATOM			A GLY Ser		43 44		6 28.635	-0.374	1.00	0.00	H
	ATOM	342	25 CZ	A SER	В	44	-15.37	5 25.028	0.346 0.255			N C
	ATOM ATOM	342 342		SER SER		44 44	-16.34! -16.513		1.167	1.00	0.15	С
20	ATOM ATOM	342		SER	В	44	-13.964	4 24.604	2.317 0.694			C C
	MOTA	342 343		SER SER		44 44	-13.788 -15.082		2.080			0
	ATOM ATOM	343	1 HA 2 1HE			44	-15.486	24.690	-0.788	1.00	0.00	H H
25	ATOM	343	3 2HB	SER		44 44	-13.183 -13.867		0.087 0.561		0.00 0.00	H H
	MOTA MOTA	343 343		SER LEU		44 45	-13.580 -17.025	25.804	2.177	1.00	0.00	H
	ATOM	343	6 CA	LEU	В	45	-17.997	22.626	0.666 1.465		0.35 0.35	N C
30	ATOM ATOM	343 343		LEU		45 45	-17.255 -16.195		2.504	1.00	0.35	С
	ATOM ATOM	343		LEU	В	45	-18.886	21.676	0.622	1.00 1.00	0.35 0.35	o C
	ATOM	344 344		LEU 1 LEU		45 45	-20.000 -20.847		1.345 0.328	1.00 1.00	0.35 0.35	С
35	ATOM ATOM	344: 344:		2 LEU LEU		45	-19.465	19.928	2.433	1.00	0.35	c c
	MOTA	344	4 HA			45 45	-16.840 -18.651	22.935 23.382	-0.247 1.916	1.00 1.00	0.00 0.00	H H
	MOTA ATOM	3445 3446	5 1HB 5 2HB	LEU :		45 45	-18.218 -19.327	20.935	0.143	1.00	0.00	H
40	ATOM	344	7 HG	LEU I	В	45	-20.665	22.235 21.614	-0.212 1.840	1.00	0.00 0.00	H H
40	ATOM ATOM	3448	3 1HD:	l Leu 1 L Leu 1	B B	45 45	-21.676 -21.291	19.564 20.767	0.821	1.00	0.00	H
	ATOM	3450	3HD1	LEU I	В	45	-20.234	19.352	-0.428 -0.203	1.00 1.00	0.00 0.00	H H
4 =	MOTA MOTA	3452	2HD2	LEU I	3	45 45	-19.720 -18.389	18.886 19.861	2.158 2.575	1.00 1.00	0.00	H
45	ATOM ATOM	3453 3454	3HD2	LEU E	3	45	-20.074	20.108	3.311	1.00	0.00 0.00	H H
	ATOM	3455	CA	SER E		46 46	-17.808 -17.218	21.826 21.081	3.734 4.809	1.00	0.48 0.48	N C
	ATOM ATOM	3456 3457		SER E		46 46	-18.124 -19.320	19.925	5.078	1.00	0.48	C
50	ATOM	3458	CB	SER B		46	-17.159	20.095 21.829	5.301 6.154	1.00 1.00	0.48 0.48	O C
	ATOM ATOM	3459 3460		SER B		46 46	-16.268 -18.582	22.929 22.438	6.093 3.972	1.00	0.48	0
	ATOM ATOM	3461 3462		SER B		16	-16.185	20.797	4.554	1.00 1.00	0.00	H H
55	ATOM	3463		SER B		16 16	-16.623 -18.133	21.080 22.087	6.739 6.591	1.00 1.00	0.00	H H
	ATOM ATOM	3464 3465	hg N	SER B		16 17	-16.007	23.091	7.021	1.00	0.00	H
	ATOM	3466	CA	GLU B			-17.561 -18.248	18.708 17.483	5.029 5.316	1.00 1.00	0.44	N C
60	ATOM ATOM	3467 3468	С 0	GLU B		_	-18.453 -19.343	17.380 16.678	6.797	1.00	0.44	С
	ATOM	3469	CB	GLU B	4	7	-17.440	16.244	7.271 4.906	1.00 1.00	0.44 0.44	o C
	ATOM ATOM	3470 3471	CG CD	GLU B			-16.115 -15.396	16.136 14.878	5.662	1.00	0.44	С
65	ATOM	3472	OE1	GLU B	4	7	-15.858	14.260	5.203 4.206		0.44 0.44	С 0
00	ATOM ATOM	3473 3474	OE2 H	GLU B			-14.373 -16.607	14.517 18.583	5.844 4.722	1.00	0.44 0.00	01-
	ATOM ATOM	3475 3476	HA 1UD	GLU B	4	7 -	-19.239	17.485	4.833	1.00	0.00	H H
7.0	ATOM	3477	2HB	GLU B	4	_	-17.273 -18.068	16.281 15.358	3.815 5.110		0.00 0.00	H H
70	MOTA MOTA	3478 3479		GLU B	4	7 -	-16.248	16.052	6.752	1.00	0.00	H
	-24 027	J 7 1 7	2115	GLU B	4	, -	-15.450	16.998	5.494	1.00	0.00	H

202

	MOTA MOTA MOTA	348	1 CA	GLU GLU	В	48 48 48	-17.41	9 17.98	8.969	1.0	0.45	N C C
5	ATOM ATOM ATOM	348 348 348	4 CB 5 CG		В	48 48 48	-16.41	7 17.28° 4 19.03°	7 10.69	7 1.00 3 1.00	0.45 0.45	0 0
1.0	ATOM ATOM ATOM	348 348 348	7 OE 8 OE	1 GLU 2 GLU	B	48 48 48	-15.749 -14.717 -15.917	7 20.938 7 22.64	9.560 3 10.099	1.00	0.45	c o o1-
10	ATOM ATOM ATOM) HA 1 1HB	GLU	B B	48 48 48	-16.949 -17.016 -15.437	16.981	9.188	1.00	0.00	H H H
15	ATOM ATOM ATOM	3493 3494	2 2HB 3 1HG 4 2HG	GLU GLU	B B	48 48 48	-16.290 -17.656 -17.412	20.717	9.869 8.238	1.00	0.00	H H H
	MOTA MOTA MOTA MOTA	3495 3496 3497 3498	CA C	THR THR THR	B B	49 49 49	-19.523 -20.475 -21.869	19.275 19.563	10.695 10.218	1.00	0.55	N C C
20	ATOM ATOM ATOM	3499 3500 3501	CB OG1	THR THR THR	B B	49 49 49 49	-22.124 -20.062 -20.882 -20.139	20.399 20.478	11.603 12.757	1.00 1.00	0.55 0.55	0 0 0
25	ATOM ATOM ATOM	3502 3503 3504	H HA	THR THR THR	B B	49 49 49	-19.450 -20.596 -19.051	19.828 18.355	10.795 8.907 11.285 11.919	1.00 1.00 1.00	0.00	С Н Н
	MOTA MOTA MOTA	3507	1HG2 2HG2	THR THR THR	B B B	49 49 49	-20.702 -19.326 -20.226	21.317 22.416 21.509	13.210 10.800 9.715	1.00 1.00 1.00		H H H H
30	ATOM ATOM ATOM	3509 3510	CA	ASN ASN	B B	49 50 50	-21.061 -22.808 -24.216	22.206 19.535 19.765	11.101 11.191 11.036	1.00 1.00 1.00	0.00 0.44 0.44	H N C
35	ATOM ATOM ATOM ATOM	3511 3512 3513 3514	C O CB	ASN ASN ASN	B B	50 50	-24.526 -23.788 -25.082	21.176 22.110 18.854	11.431 11.124 11.923	1.00 1.00 1.00	0.44 0.44 0.44	с 0 с
	ATOM ATOM ATOM	3514 3515 3516 3517		ASN ASN ASN ASN	B B	50 50 50 50	-24.987 -25.306 -24.536 -22.432	17.436 17.184 16.483 19.612	11.383 10.223 12.243	1.00 1.00 1.00	0.44 0.44	С О И
40	ATOM ATOM ATOM	3518 3519 3520	HA 1HB	ASN ASN ASN	B B	50 50 50	-24.490 -26.160 -24.811	19.648 19.052 18.926	12.132 9.974 11.801 12.988	1.00 1.00 1.00 1.00	0.00 0.00 0.00	H H H
4.5	ATOM ATOM ATOM	3521 3522 3523		ASN ASN SER	В	50 50 51	-24.229 -24.434 -25.661	16.692 15.557 21.345	13.173 11.862 12.140	1.00 1.00 1.00	0.00 0.00 0.25	H H N
45	ATOM ATOM ATOM	3524 3525 3526	CA C O	SER I	В	51 51 51	-26.182 -25.171 -24.943	22.633 23.418 24.590	12.494 13.267 12.969	1.00 1.00 1.00	0.25 0.25 0.25	C C
50	ATOM ATOM ATOM	3527 3528 3529	CB OG H	SER I	B B .	51 51 51	-27.446 -27.126 -26.217	22.542 21.972 20.565	13.365 14.625 12.448	1.00 1.00 1.00	0.25 0.25 0.00	С О Н
	ATOM ATOM ATOM	3530 3531 3532	2HB	SER I	3 .		-26.415 -28.208 -27.883	23.201 21.903 23.550	13.489	1.00 1.00 1.00	0.00	H H H
55	ATOM ATOM ATOM ATOM	3533 3534 3535 3536		SER I SER I SER I	3 .	52 52	-26.652 -24.525 -23.591	22.654 22.810 23.593	15.134 14.278 15.036	1.00 1.00 1.00	0.00 0.14 0.14	H N C
60	ATOM ATOM ATOM	3537 3538 3539	O CB	SER E SER E SER E SER E	3 5	52 52	-22.214 -21.944 -23.794 -25.058	23.106 21.906 23.486 24.020	14.740 14.768 16.557	1.00 1.00 1.00	0.14 0.14 0.14	с о с
	ATOM ATOM ATOM	3540 3541	H HA	SER B SER B SER B		52 52	-24.570 -23.702 -22.979	21.822 24.662 24.029	16.919 14.458 14.810 17.070	1.00 1.00 1.00 1.00	0.14 0.00 0.00 0.00	О Н Н
65	ATOM ATOM ATOM	3543 3544 3545	2HB HG	SER B SER B LEU B	5	52 52	-23.770 -24.950 -21.296	22.444 24.982 24.040	16.905 16.985 14.422	1.00 1.00 1.00	0.00 0.00 0.00	н н н N
70	ATOM ATOM ATOM	3546 3547 3548	CA : C : O :	LEU B LEU B LEU B	5 5	3 3	-19.948 -19.099 -19.090	23.630 24.280 25.503	14.179 15.218 15.358	1.00 1.00 1.00	0.09 0.09 0.09	c c o
70	ATOM ATOM	3549 3550		LEU B LEU B			-19.400 -17.946	24.033 23.579	12.798	1.00	0.09	C

	ATO	M 3552	CD1 :	LEU I	3 5			19 12.59 12 11.25		0.09	c c
5	ATOM ATOM ATOM	4 3554 4 3555	HA 1	LEU I LEU I	3 5	3 -19.8	97 25.03 73 22.54	7 14.37 5 14.29	8 1.00 2 1.00	0.00	H H
	AOTA AOTA AOTA	4 3557		LEU E LEU E	3 53	3 -17.33	06 23.75 35 23.99	4 12.01 6 13.37	4 1.00 7 1.00	0.00 0.00 0.00	H H H
10	ATOM ATOM ATOM	1 3559 1 3560	2HD1 I 3HD1 I 1HD2 I	EU B	53	3 -18.52 3 -17.75	21 21.53 34 21.59	5 13.25° 4 11.60°	7 1.00	0.00 0.00 0.00	H H H
	ATOM ATOM ATOM	3562 3563	2HD2 I 3HD2 I	EU B	53 53	-17.86 -17.54	22 23.76 4 25.26	5 10.34	1.00	0.00 0.00 0.00	н н н
15	MOTA MOTA	3565 3566	CA A	SN B SN B SN B	54 54 54	-17.52	9 24.01	2 17.013	1.00	0.09 0.09 0.09	N C C
20	MOTA MOTA MOTA	3568 3569	CB A	SN B SN B SN B	54 54 54	-17.80	9 22.471 0 23.445	l 16.374	1.00	0.09 0.09	o c
20	ATOM ATOM ATOM	3571	OD1 A ND2 A H A		54 54 54	-16.40 -16.91 -18.26	9 25.286 6 23.767	19.069 20.679	1.00 1.00	0.09 0.09 0.09	C O N
25	ATOM ATOM MOTA	3573 3574 : 3575 :	HA A	SN B SN B SN B	54 54 54	-17.68; -17.55; -18.86	2 25.091 5 22.373	17.053 18.473	1.00 1.00	0.00 0.00 0.00	H H H
	ATOM ATOM ATOM	3576	HD2 AS	N B	54 54	-17.372 -16.360	2 22.916 2 24.293	20.949 21.330	1.00 1.00 1.00	0.00 0.00 0.00	H H H
, 30	ATOM ATOM ATOM	3579 3580 3581	CA II	E B	55 55 55	-15.213 -13.854 -13.041	24.291 24.735	16.677 16.377 17.542	1.00 1.00 1.00	0.08 0.08 0.08	И С С
	MOTA MOTA MOTA	3582 3583	CB II		55 55 55	-13.336 -13.310 -13.293	25.010 26.527	18.178 15.178 15.424	1.00 1.00 1.00	80.0 80.0 80.0	0 0
35	MOTA MOTA	3586		E B E B	55 55 55	-14.135 -12.481 -15.436	27.296 25.536	13.950 14.384 17.039	1.00 1.00 1.00	0.08 0.08 0.00	C C
40	ATOM ATOM ATOM	3588 3589 1	HB IL HG1 IL	e b e b	55 55 55	-13.731 -12.270 -12.814	24.659 26.841	16.238 15.038 16.356	1.00 1.00	0.00 0.00 0.00	н н н
40	ATOM ATOM ATOM	3590 2: 3591 1: 3592 2:	HG2 IL HG2 IL	e b e b	55 55 55	-14.341 -13.703 -14.181	26.851 24.971 23.491	15.420 13.010 13.855	1.00	0.00 0.00 0.00	H H H
45	ATOM ATOM ATOM	3594 11 3595 21	ID1 ILI	E B E B	55 55 55	-15.169 -12.528 -11.433	24.966 28.384 26.989	14.004 14.547 14.474	1.00	0.00	H H
	ATOM ATOM ATOM	3596 31 3597 1 3598 0		В	55 56 56	-12.805 -11.988 -11.128	27.104 23.964 24.307	13.349 17.855 18.942	1.00 (0.00	H H N
50	atom atom atom		VAI B VAI	B	56 56 56	-9.803 -9.483 -10.938	24.597 24.091 23.177	18.333 17.259 19.914	1.00 0	0.10 0.10 0.10	С С
	ATOM ATOM ATOM	3602 C 3603 C 3604 H	G1 VAI G2 VAI VAL	В		-9.887 -12.308 -11.643	23.579 22.813 23.243	20.962 20.510	1.00 0 1.00 0	.10 .10 .10	c c
55	ATOM ATOM ATOM	3605 H 3606 H 3607 1H	A VAL	B B	56 56	-11.486 -10.550 -10.078	25.247 22.293	17.244 19.322 19.374	1.00 0 1.00 0	.00	H H H
60	ATOM ATOM ATOM	3608 2H 3609 3H 3610 1H	G1 VAL G1 VAL	B !	56 56	-8.900 -9.712	23.069 23.203 24.626	21.922 20.639 21.212	1.00 0	.00 .00 .00	H H H
	ATOM ATOM MOTA	3611 2H0 3612 3H0 3613 N	G2 VAL	B 5	56 - 56 -	-12.215 -12.874 -12.944	22.112 23.684 22.313	19.759	1.00 0	.00 .00 .00	H H H
65	ATOM ATOM ATOM	3614 C	A ASN ASN	B 5	57 57 57	-9.004 -7.708 -7.819	25.802 26.255	18.547	1.00 0.	.11 .11 .11	N C C
	ATOM ATOM	3616 O 3617 CE 3618 CG	ASN	B 5	7	-7.234 -6.662 -5.291	24.678	16.227 18.634	1.00 0. 1.00 0.	11 11 11	0 C
70			01 ASN 02 ASN ASN	B 5	_	-4.310	24.880	17.634 1 19.303 1	1.00 0. 1.00 0.	11 11	O N H

	ATON ATON ATON	4 362	23 1HE	3 ASN	В	57	-6.80	7 23.90	6 17.86			
	ATOM			3 ASN 32 ASN	B	57 57						
5	ATOM	1 362		2 ASN	В	57						
	ATOM			ALA		58		3 27.32	6 16.89			H N
	ATOM ATOM					58			9 15.55			c
	ATOM			ALA ALA		58 58						С
10	ATOM					58						0
	ATOM			ALA		58	-9.19					C
	ATOM					58	-9.15					H H
	ATOM	-	4 1HB			58	-9.72		6 14.36			H
15	ATOM ATOM			ALA ALA		58 58	-10.589					Н
	ATOM			LYS		59	-9.110 -6.97					H
	ATOM			LYS		59	-5.653					N
	ATOM			LYS		59	-5.67	29.20				C
20	MOTA MOTA			LYS		59	-6.710					ō
20	ATOM	3642		LYS LYS		59 59	-5.066					С
	MOTA	3643		LYS		59	-4.819 -3.812			_		С
	ATOM	3644	1 CE	LYS		59	-3.593					C
25	ATOM	3645		LYS		59	-2.607	24.846			0.31	C N1+
23	ATOM ATOM	3646 3647		LYS		59	-7.667		13.284		0.00	Н
	ATOM		HA HB	LYS LYS		59 59	-4.994 -4.188				0.00	H
	ATOM		2HB	LYS		59	-5.917				0.00	H
3.0	MOTA		1HG	LYS		59	-4.449			1.00	0.00	H
30	ATOM		2HG	LYS		59	-5.784	25.249		1.00	0.00	H H
	ATOM ATOM		1HD 2HD	LYS		59	-4.154		15.231	1.00	0.00	H
	ATOM		1HE	LYS LYS		59 59	-2.851 -3.202			1.00	0.00	H
	ATOM	3655		LYS		59	-4.527	23.717 24.225	14.846 15.925	1.00	0.00	H
35	ATOM	3656	1HZ	LYS		59	-2.435	24.037	17.091	1.00	0.00 0.00	H
	MOTA	3657		LYS		59	-1.719	25.149	16.136	1.00	0.00	H H
	ATOM ATOM	3658	3HZ	LYS		59	-2.973	25.567	17.120	1.00	0.00	H
	ATOM	3659 3660	N CA	PHE I		60 60	-4.477	29.552	11.983	1.00	0.23	N
40	ATOM	3661	c	PHE I		60	-4.318 -5.095	30.638 30.287	11.063	1.00	0.23	C
	ATOM	3662	0	PHE I		60	-5.704	31.140	9.839 9.197	1.00 1.00	0.23 0.23	C O
	ATOM	3663	CB	PHE I		60	-2.858	30.850	10.632	1.00	0.23	c
	ATOM ATOM	3664 3665	CG CD1	PHE E		60	-2.873	31.832	9.510	1.00	0.23	Č
45	ATOM	3666		PHE E		60 60	-2.961 -2.798	33.184 31.391	9.748	1.00	0.23	С
	ATOM	3667		PHE E		60	-2.977	34.079	8.208 8.705	1.00 1.00	0.23 0.23	C
	ATOM	3668		PHE B		60	-2.813	32.282	7.161	1.00	0.23	C
	ATOM	3669	CZ	PHE B		60	-2.902	33.630	7.409	1.00	0.23	Ċ
50	ATOM ATOM	3670 3671	H HA	PHE B		60 60	-3.633	29.102	12.295	1.00	0.00	н
	ATOM	3672	1HB	PHE B		60	-4.520 -2.378	31.613 29.909	11.406 10.321	1.00	0.00	H
	ATOM	3673		PHE B		60	-2.278	31.227	11.490	1.00 1.00	0.00	H
	ATOM	3674		PHE B		60	-3.027	33.553	10.769	1.00	0.00	H H
55	MOTA MOTA	3675 3676		PHE B		60	-2.735	30.326	7.999	1.00	0.00	H
	ATOM	3677		PHE B PHE B		60 60	-3.056	35.145	8.908	1.00	0.00	H
	ATOM	3678		PHE B		50	-2.763 -2.922	31.919 34.338	6.138 6.584	1.00	0.00	H
	ATOM	3679		GLU B		51	-5.095	28.987	9.508	1.00 1.00	0.00 0.15	H N
60	ATOM	3680		GLU B		51	-5.748	28.446	8.354	1.00	0.15	C
00	ATOM	3681		GLU B		1	-7.218	28.714	8.459	1.00	0.15	č
	ATOM ATOM	3682 3683		GLU B		1	-7.889	28.938	7.454	1.00	0.15	0
	ATOM	3684		GLU B		1	-5.528 -5.975	26.930	8.259		0.15	C
	ATOM	3685		GLU B		1	-5.349	26.190 24.803	9.522 9.510	1.00	0.15	C
65	ATOM	3686	OE1	SLU B		1	-5.260	24.199	8.408		0.15 0.15	C 0
	ATOM	3687	OE2			1	-4.938	24.333	10.605		0.15	01-
	ATOM ATOM	3688 3689		FLU B		1	-4.636	28.314	10.097	1.00	0.00	н
	ATOM	3690 1		FLU B	6	1 1	-5.382 -4.456	28.950	7.445		0.00	H
70	ATOM	3691 2	HB G	LU B	6			26.737 26.577			0.00 0.00	H
	ATOM	3692 1	HG G	LU B	6			26.116			0.00	H H

5	ATON ATON ATON ATON ATON ATON	4 3694 4 3695 4 3696 4 3697 4 3698 4 3699	N ASP II CA ASP II C ASP II O ASP II CB ASP II CG ASP II	3 62 3 62 3 62 3 62 3 62	-7.75 -9.16 -9.66 -10.82 -9.53 -9.41	51 28.719 50 28.869 54 30.184 8 30.280 9 28.746 3 27.276	9.699 9.932 9.423 9.042 5 11.419	1.00 2 1.00 1 1.00 1 1.00 3 1.00	0.16 0.16 0.16 0.16 0.16	н с с с
10	ATOM ATOM ATOM ATOM	3701 3702 3703 3704 1	OD1 ASP E OD2 ASP E H ASP B HA ASP B HB ASP B	62 62 62 62		5 26.952 2 28.495 2 28.115	13.000 10.507 9.343	1.00 1.00 1.00		О О1- Н Н
15	ATOM ATOM ATOM ATOM	3706 3707 3708 3709	HB ASP B N SER B CA SER B C SER B C SER B	63 63	-9.01 -8.83 -9.30 -9.86 -9.32	2 31.244 8 32.524 9 32.382	9.415	1.00 1.00 1.00	0.00 0.20 0.20 0.20 0.20	H N C C
20	ATOM ATOM ATOM ATOM ATOM	3711 (3712 F	CB SER B CG SER B H SER B HA SER B HB SER B	63 63 63 63	-8.213 -7.222 -7.856 -10.093 -7.772	33.604 33.255 31.085 32.837	8.921 7.966 9.622 9.673 9.916	1.00 1.00 1.00 1.00	0.20 0.20 0.00 0.00	С Н Н
25	ATOM ATOM ATOM ATOM	3717 N	IB SER B IG SER B I GLY B IA GLY B	63 63 64 64	-8.648 -6.730 -11.016 -11.651 -13.081	34.553 32.485 33.050 32.974	8.584 8.307 7.328 6.044 6.233	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.22 0.22	H H H N C
30	ATOM ATOM ATOM ATOM ATOM	3720 O 3721 H 3722 1H 3723 2H 3724 N	GLY B GLY B A GLY B A GLY B	64 64 64 65	-13.461 -11.410 -11.495 -11.200 -13.918	33.869 33.693 32.015 33.716	7.288 8.006 5.554 5.359	1.00 1.00 1.00 1.00	0.22 0.22 0.00 0.00 0.00	С О Н Н
35	MOTA MOTA MOTA MOTA MOTA	3725 C. 3726 C 3727 O 3728 C! 3729 C	GLU B GLU B GLU B	65 65 65 65	-15.307 -16.074 -15.711 -15.910	33.483 32.222 31.164 34.122	5.199 5.302 5.515 5.000 4.040	1.00 1.00 1.00 1.00	0.19 0.19 0.19 0.19 0.19	и С О С
40	ATOM ATOM ATOM ATOM ATOM	3730 CI 3731 OI	GLU B E1 GLU B E2 GLU B GLU B	65 65 65 65	-15.403 -16.200 -16.409 -16.625 -13.592	35.529 36.045 35.260 37.231 32.750	3.730 2.539 1.575 2.584 4.322	1.00 1.00 1.00 1.00	0.19 0.19 0.19 0.19 0.00	С С О О1- Н
45	ATOM ATOM ATOM ATOM ATOM	3735 1HE 3736 2HE 3737 1HG 3738 2HG 3739 N	GLU B GLU B GLU B	65 65 65	-15.418 -16.996 -15.743 -14.334 -15.576	34.200 34.170 33.449 35.505 36.196	6.112 4.211 3.182 3.473 4.587	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н н
50	MOTA MOTA MOTA	3740 CA 3741 C 3742 O 3743 CB	TYR B TYR B TYR B	66 66 66	-17.164 -17.970 -19.342 -19.839 -18.124	32.306 31.148 31.425 32.548 30.795	6.304 6.549 6.020 6.099 8.040	1.00 1.00	0.22 0.22 0.22 0.22 0.22	и С С С
55	ATOM ATOM ATOM ATOM ATOM ATOM	3746 CD 3747 CE	TYR B 1 TYR B 2 TYR B 1 TYR B 2 TYR B TYR B	66 66 66	-16.782 -15.918 -16.382 -14.679 -15.144 -14.291	30.418 31.384 29.102 31.041 28.752 29.723	8.567 9.033 8.592 9.522 9.078 9.544	1.00 1.00 1.00 1.00 1.00	0.22 0.22 0.22 0.22 0.22	00000
60	ATOM ATOM ATOM ATOM ATOM	3750 OH 3751 H 3752 HA 3753 1HB 3754 2HB	TYR B TYR B TYR B TYR B	66 - 66 - 66 -	-13.021 -17.342 -17.532 -18.806	29.367 33.146 30.275 29.929	10.044 6.847 6.047 8.084	1.00 (1.00 (1.00 (1.00 (0.22 0.22 0.00 0.00	С О Н Н
65	ATOM ATOM ATOM ATOM ATOM	3755 HD2 3756 HD2 3757 HE1 3758 HE2	TYR B TYR B TYR B	66 - 66 - 66 -	-18.599 -16.191 -17.046 -13.997 -14.837	31.552 32.433 28.325 31.799 27.708	9.006 8.221 9.847	1.00 0 1.00 0	0.00 0.00 0.00 0.00	H H H H
70	ATOM ATOM ATOM ATOM	3759 HH 3760 N 3761 CA 3762 C 3763 O	LYS B C	57 - 57 - 57 -	21.299	29.749 30.391 30.533 29.279 28.239	5.440 4.900 5.238	1.00 0 1.00 0 1.00 0	.00 .45 .45 .45	H N C C

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	ATOM ATOM	376 376				67 67			3.37			C
	ATOM					67			2.871 1.394			C
r.	ATOM					67			1.129			c
5	MOTA MOTA	376				67			1.761			N1+
	ATOM	3769 3770		LYS LYS		67 67			5.412			Н
	ATOM		l 1HB			67			5.361 3.016			H
1.0	ATOM		2 2HB	LYS		67			2.952			H H
10	MOTA		3 1HG			67			3.468		0.00	H
	MOTA MOTA		2HG			67			3.088		0.00	H
	MOTA		2HD			67 67	-19.999 -21.053		0.954 0.812		0.00	H
	ATOM		7 1HE			67	-18.775		0.049		0.00	H H
15	ATOM		2HE			67	-19.097	29.947	1.529		0.00	н
	MOTA MOTA		Hz 2Hz	LYS		67	-16.926		1.480		0.00	H
	ATOM		3HZ	LYS LYS		67 67	-17.675 -17.826		1.507		0.00	H
	MOTA	3782		CYS		68	-23.383		2.772 5.281	1.00	0.00 0.52	H N
20	MOTA	3783		CYS	В	68	-24.163		5.606		0.52	Č
	ATOM	3784		CYS		68	-25.428	28.222	4.811	1.00	0.52	č
	ATOM ATOM	3785 3786		CYS CYS		68	-25.970	29.288	4.524	1.00	0.52	0
	ATOM	3787		CYS		68 68	-24.621 -25.956	28.179 26.981	7.065 7.311	1.00	0.52	C
25	ATOM	3788		CYS		68	-23.896	30.171	5.002	1.00	0.52	s H
	ATOM	3789		CYS		68	-23.591	27.287	5.374	1.00	0.00	H
	ATOM	3790		CYS		68	-24.992	29.178	7.349	1.00	0.00	н
	MOTA ATOM	3791 3792		CYS GLN		68 69	-23.803 -25.931	27.921	7.723	1.00	0.00	H
30	ATOM	3793	CA	GLN		69	-27.206	27.034 27.001	4.420 3.771	1.00	0.27 0.27	N
	MOTA	3794	С	GLN		69	-27.926	25.780	4.234	1.00	0.27	C
	ATOM	3795	0	GLN		69	-27.323	24.828	4.727	1.00	0.27	ō
	ATOM ATOM	3796 3797	CB CG	GLN GLN		69	-27.150	26.927	2.237	1.00	0.27	С
35	ATOM	3798	CD	GLN		69 69	-26.530 -26.687	25.639 25.656	1.700 0.186	1.00	0.27	C
	ATOM	3799		GLN		69	-27.435	26.466	-0.360	1.00	0.27 0.27	С 0
	ATOM	3800		GLN		69	-25.967	24.736	-0.511	1.00	0.27	N
	ATOM ATOM	3801	H	GLN		69	-25.524	26.151	4.696	1.00	0.00	H
40	ATOM	3802 3803	HA 1HB	GLN GLN		69 69	-27.798 -26.598	27.874 27.802	4.081	1.00	0.00	H
	ATOM	3804		GLN		69	-28.189	27.025	1.859 1.876	1.00	0.00	H H
	ATOM	3805		GLN		69	-27.185	24.835	2.029	1.00	0.00	H
	ATOM ATOM	3806		GLN GLN	В	69	-25.497	25.492	2.036	1.00	0.00	H
45	ATOM	3808				69 69	-25.235 -25.927	24.219	-0.068	1.00	0.00	Н
	ATOM	3809	N	HIS		70	-29.263	24.943 25.803	-1.496 4.102	1.00 1.00	0.00 0.11	H N
	MOTA	3810	CA	HIS		70	-30.076	24.678	4.443	1.00	0.11	C
	ATOM	3811	С	HIS		70	-30.899	24.396	3.237	1.00	0.11	C
50	ATOM ATOM	3812 3813	O CB	HIS HIS		70	-30.877	25.150	2.267	1.00	0.11	0
-	ATOM	3814	CG	HIS		70 70	-31.043 -30.339	24.920 24.997	5.612 6.930	1.00	0.11 0.11	C
	MOTA	3815		HIS		70	-29.937	23.891	7.646	1.00	0.11	C N
	ATOM	3816		HIS		70	-29.953	26.075	7.664	1.00	0.11	Ċ
55	ATOM ATOM	3817		HIS		70	-29.331	24.351	8.768	1.00	0.11	С
55	ATOM	3818 3819	H H	HIS :		70 70	-29.316 -29.699	25.671 26.490	8.824	1.00	0.11	N
	ATOM	3820	HA	HIS		70	-29.447	23.799	3.501 4.660	1.00 1.00	0.00	H H
	ATOM	3821	1HB	HIS I		70	-31.766	24.089	5.657	1.00	0.00	H
60	ATOM		2HB	HIS I		70	-31.637	25.829	5.471	1.00	0.00	H
00	ATOM ATOM	3823 3824		HIS I		70	-30.099	27.123	7.447	1.00	0.00	H
	ATOM	3825	HE2	HIS I	P B	70 70	-29.020 -29.018	23.707 26.241	9.580 9.593	1.00	0.00	H
	ATOM	3826	N	GLN I		71	-31.625	23.266	3.251	1.00	0.00 0.12	H N
C E	ATOM	3827	CA	GLN I	3	71	-32.441	22.954	2.121	1.00	0.12	C
65	ATOM	3828	C	GLN H		71	-33.468	24.032	2.009	1.00	0.12	С
	MOTA MOTA	3829 3830	O CB	GLN E		71 71	-33.753 -33.197	24.525	0.920		0.12	0
	ATOM	3831	CG	GLN E		71	-33.197	21.623 20.379	2.276 2.279	1.00	0.12 0.12	C C
70	ATOM	3832	CD	GLN E	3		-31.895	20.083	0.843		0.12	c
70	ATOM	3833		GLN E		71	-32.123	20.883	-0.063	1.00	0.12	ŏ
	ATOM	3834	NE2	GLN E	3	71	-31.272	18.896	0.623		0.12	N

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	ATON ATON	383			В	71 71	~31.83	4 22.97	7 1.20	4 1.0		
5	ATOM	383	8 2HB	GLN	В	71 71			15 1.46 4 3.22			
5	ATOM ATOM		9 1HG			71 71		4 19.51	9 2.66	8 1.0	0.00	н с
	ATOM ATOM	384	1 1HE	2 GLN	В	71	-31.12	5 18.25	2 1.39			
1.0	ATOM		2 2HE 3 N	2 GLN GLN		71 72						H
10	ATOM ATOM				В	72	-35.11	7 25.37	7 3.18	8 1.0		
	ATOM	384	6 0	GLN GLN		72 72	-34.66 -35.30					
	ATOM ATOM			GLN GLN		72 72	-35.69	25.54	6 4.60	2 1.0	0 0.21	. с
15	ATOM	384	9 CD	GLN	В	72	-36.10 -37.05				_	
	MOTA MOTA			GLN GLN		72 72	-37.630 -37.224	24.08	2 3.40	0 1.0	0 0.21	0
	ATOM	385	2 H	GLN	В .	72	-33.776					
20	MOTA MOTA	3853 3854	3 HA 4 1HB	GLN GLN		72 72	-35.857 -36.568		2.43	3 1.0	0.00	
	ATOM	3855	5 2HB	GLN	В	72	-34.952					H H
	ATOM ATOM		5 1HG 7 2HG	GLN GLN		72 72	-36.614 -35.212		6.21	1.00	0.00	H
25	MOTA	3858	3 1HE2	GLN	в 7	72	-36.791					H H
25	MOTA MOTA	3859 3860		GLN VAL		72 73	-37.890 -33.516		3.966	1.00	0.00	H
	ATOM	3861	CA	VAL	в 7	3	-33.130					N C
	MOTA MOTA	3862 3863		VAL :		3	-32.145 -31.658	28.702	1.959	1.00	0.31	С
30	ATOM	3864	CB	VAL 1	3 7	3	-32.521					o c
	ATOM ATOM	3865 3866		VAL I		3	~33.583		5.395	1.00	0.31	С
	MOTA	3867	H	VAL I	3 7	3	-31.247 -32.902	28.442 26.625	4.666 3.835			C H
35	ATOM ATOM	3868 3869		VAL I			-34.032 -32.166	29.136	2.786	1.00	0.00	H
	ATOM	3870	1HG1	VAL E	3 7		-33.219	30.225 29.820	4.101 6.275	1.00	0.00	H H
	ATOM ATOM	3871 3872	2HG1	VAL E	3 7: 3 7:		-34.505	29.762	5.053	1.00	0.00	H
40	ATOM	3873	1HG2	VAL E	7:		-33.855 -31.260	28.254 28.169	5.740 5.729	1.00	0.00 0.00	H H
40	ATOM ATOM	3874 3875	2HG2	VAL E	7:		-31.174 -30.331	27.490	4.129	1.00	0.00	H
	ATOM	3876	N	ASN B	74		-31.857	28.965 29.979	4.407 1.634	1.00	0.00 0.41	H N
	MOTA MOTA	3877 3878	CA C	ASN B			-30.932 -29.580	30.413	0.630	1.00	0.41	С
4 5	ATOM	3879	0	ASN B	74	1	-29.409	30.362 29.751	1.270 2.322	1.00	0.41 0.41	С 0
	ATOM ATOM	3880 3881	CB CG	ASN B	74		-31.202 -30.458	31.869	0.200	1.00	0.41	С
	ATOM	3882	OD1	ASN B	74	ı	-29.812	32.179 31.313	-1.090 -1.676	1.00	0.41 0.41	C O
50	ATOM ATOM	3883 3884		ASN B ASN B	74 74	l l	-30.542 -32.331	33.459 30.717	-1.542	1.00	0.41	N
	ATOM	3885	HA	ASN B	74		-30.976	29.713	2.145 -0.222	1.00 1.00	0.00 0.00	H H
	MOTA MOTA	3886 3887		ASN B ASN B	74 74		-30.921 -32.278	32.561 32.002	1.004	1.00	0.00	H
55	ATOM	3888	1HD2	ASN B	74		-30.976	34.179	-0.003 -0.997	1.00 1.00	0.00 0.00	H H
JJ	ATOM ATOM	3889 3890	2HD2	ASN B	74 75		-29.971 -28.567	33.687 30.970	-2.339	1.00	0.00	H
	ATOM	3891	CA	GLU B	75		-27.249	31.003	0.622 1.180	1.00 1.00	0.48 0.48	N C
	ATOM ATOM	3892 3893		GLU B	75 75		-27.241 -27.925	32.069 33.085	2.228	1.00	0.48	С
60	ATOM	3894	CB (GLU B	75	-	-26.170	31.366	2.100 0.145	1.00 1.00	0.48 0.48	o c
	ATOM ATOM	3895 3896		GLU B	75 75		-26.047 -25.367	30.340 29.103	-0.982	1.00	0.48	С
	MOTA	3897	OE1	SLU B	75	-	-24.699	29.229	-0.418 0.643	1.00	0.48 0.48	С О
65	ATOM ATOM	3898 3899	OE2 O	FLU B	75 75		-25.503	28.015	-1.039	1.00	0.48	01-
	ATOM	3900	HA C	LU B	75		-28.657 -27.017	31.252 30.019	-0.347 1.621	1.00	0.00	H H
	ATOM ATOM	3901 1 3902 2		LU B	75 75		25.207	31.519	0.665	1.00	0.00	H
70	ATOM	3903 1	LHG G	LU B	75		26.423 25.416	32.357 30.732	-0.272 -1.797	1.00	0.00	H H
70	ATOM ATOM	3904 2 3905		LU B ER B	75 76		27.009	30.079	-1.450	1.00	0.00	H
				5	, 0	_	26.469	31.848	3.309	1.00	0.42	N

	ATO ATO			SER SER		76 76						
	ATO	1 3908		SER		76						_
5	ATO			SER	В	76	-25.95					
5	ATON ATON		OG	SER		76	-25.87		3 6.72			
	ATOM		H HA	SER SER		76 76	-26.02 -27.34) H
	ATON			SER		76	-24.91			_		
1.0	ATO			SER		76	-26.36					
10	ATOM		HG	SER		76	-25.07	6 33.68				
	ATOM ATOM		N CA	GLU		77	-25.36					
	ATOM		C	GLU		77 77	-24.35 -23.10					. С
	ATOM		ō	GLU		 77	-23.10					-
15	ATOM		CB	GLU		77	-24.59		5.02			
	ATOM		CG	GLU		77	-25.87	8 38.032				c
	ATOM ATOM		CD OF1	GLU GLU		77	-26.98			-		č
	MOTA			GLU		77 77	-26.70° -28.12°					0
20	ATOM		Н	GLU :		7	-26.10			_		01-
	MOTA	3926	HA	GLU I	В 7	7	-24.35					H H
	ATOM		1HB	GLU I		7	-23.730	37.950				H
	MOTA MOTA	3928 3929	2HB 1HG	GLU I		7	-24.496					н
25	ATOM	3930		GLU I		7	-26.103 -25.778			_		H
	ATOM	3931	N	PRO I			-22.004		4.71			H
	ATOM	3932	CA	PRO E		8	-20.764		4.932			N C
	ATOM ATOM	3933	C	PRO E			-20.323		6.15			Ċ
30	ATOM	3934 3935	O CB	PRO E			~20.684		6.323		0.29	Ö
	ATOM	3936	CG	PRO E			-19.756 -20.627		3.788		– •	С
	ATOM	3937	CD	PRO E			-21.979		2.527			C
	ATOM	3938	HA	PRO B			-20.930	34.229	5.154			C H
35	ATOM ATOM	3939 3 3940 2		PRO B			-18.975	34.595	3.881			H
	ATOM	3941 1		PRO B			-19.253	36.340	3.777			H
	ATOM	3942 2	HG	PRO B	78		-20.743 -20.192	34.219 35.781	2.155 1.679			H
	ATOM	3943 1		PRO B	78		-22.062	36.874	2.622	1.00	0.00 0.00	H H
40	ATOM	3944 2		PRO B	78		-22.791	35.253	2.482	1.00	0.00	H
40	ATOM ATOM	3945 3946		VAL B VAL B	79		-19.557	35.337	7.022	1.00	0.31	N
	ATOM			VAL B	79 79		-18.978 -17.507	35.931 35.760	8.187	1.00	0.31	С
	MOTA			VAL B	79		-17.055	34.693	8.006 7.593	1.00	0.31	С
45	ATOM			VAL B	79		-19.362	35.248	9.465	1.00	0.31 0.31	o C
40	ATOM ATOM	3950	CG1	VAL B	79		-18.925	33.776	9.386	1.00	0.31	c
	ATOM			VAL B	79 79		-18.732	36.018	10.638	1.00	0.31	C
	ATOM			VAL B	79		-19.361 -19.257	34.360 36.997	6.860	1.00	0.00	H
E O	ATOM		HB V	VAL B	79		-20.462	35.289	8.216 9.567	1.00	0.00 0.00	H H
50	ATOM ATOM	3955 1	HG1 V	/AL B	79		-19.391	33.205	10.210	1.00	0.00	н
	ATOM	3956 21 3957 31	HG1 \	/AL B	79		-19.283	33.319	8.460	1.00	0.00	H
	ATOM	3958 11	IG2 V	/ALL B	79 79		-17.846 -19.088	33.643	9.523	1.00	0.00	H
	ATOM	3959 21	IG2 V	AL B	79		-17.634	35.629 35.926	11.607 10.652	1.00	0.00	H
55	ATOM	3960 3I	IG2 V	AL B	79		18.990	37.090	10.606	1.00	0.00 0.00	H H
	ATOM ATOM			YR B	80		16.709	36.805	8.294	1.00	0.19	N
	ATOM	3962 C		YR B YR B	80		15.305	36.638	8.067	1.00	0.19	C
	ATOM	3964		YR B	80 80		14.649 14.925	36.465	9.394	1.00	0.19	С
60	ATOM		-	YR B	80		14.628	37.197 37.826	10.343 7.359	1.00	0.19	0
	ATOM			YR B	80	-	13.244	37.390	7.018	1.00	0.19 0.19	C C
	ATOM ATOM		D1 T		80		12.214	37.522	7.921	1.00	0.19	c
	ATOM	3968 C	D2 T E1 T	YR B	80		12.983	36.837	5.785	1.00	0.19	С
65	ATOM	3970 C	E2 T	YR R	80 80		10.942 11.714	37.112	7.597	1.00	0.19	С
	ATOM	3971 C		YR B	80		10.692	36.425 36.565	5.454 6.360	1.00	0.19	C
	MOTA	3972 0	H T	YR B	80		-9.387	36.143	6.025	1.00	0.19 0.19	C 0
	ATOM	3973 H		YR B	80	-:	17.008	37.682	8.682	1.00	0.00	н
70	ATOM ATOM	3974 H		YR B	80		15.133	35.776	7.415	1.00	0.00	H
	ATOM	3976 2H		YR B YR B	80 80		14.633	38.725	7.994	1.00	0.00	H
			- 1.	D	50		15.197	38.081	6.450	1.00	0.00	H

TOM 3980 HE1 TYR B 80 -10.137 37.169 8.309 ATOM 3980 HE2 TYR B 80 -11.519 36.016 4.465 ATOM 3981 HH TYR B 80 -8.978 35.822 6.837 ATOM 3982 N LEU B 81 -13.760 35.460 9.490 ATOM 3983 CA LEU B 81 -13.094 35.195 10.729 ATOM 3984 C LEU B 81 -11.635 35.443 10.529 ATOM 3985 O LEU B 81 -11.076 35.109 9.485 ATOM 3986 CB LEU B 81 -13.250 33.736 11.191 ATOM 3987 CG LEU B 81 -12.542 33.429 12.522	1.00 0.00 H 1.00 0.00 H 1.00 0.00 H 1.00 0.08 N 1.00 0.08 C 1.00 0.08 H 1.00 0.08 C
ATOM 3983 CA LEU B 81 -13.094 35.195 10.729 ATOM 3984 C LEU B 81 -11.635 35.443 10.529 ATOM 3985 O LEU B 81 -11.076 35.109 9.485 ATOM 3986 CB LEU B 81 -13.250 33.736 11.191 ATOM 3987 CG LEU B 81 -12.542 33.429 12.522	1.00 0.08 C 1.00 0.08 C 1.00 0.08 O 1.00 0.08 C 1.00 0.08 C 1.00 0.08 C 1.00 0.08 C
ATOM 3986 CB LEU B 81 -13.250 33.736 11.191 ATOM 3987 CG LEU B 81 -12.542 33.429 12.522	1.00 0.08 C 1.00 0.08 C 1.00 0.08 C 1.00 0.08 C 1.00 0.00 H
ATOM 3988 CDI LEU B 81 -13.157 34.234 13.678	1.00 0.08 C 1.00 0.00 H
ATOM 3990 H LEU B 81 -13.530 34.870 8.697 ATOM 3991 HA LEU B 81 -13.489 35.875 11.494	1 00 0 00
ATOM 3993 2HB LEU B 81 -14.319 33.473 11.257 ATOM 3994 HG LEU B 81 -11.483 33.725 12.421 ATOM 3995 1HD1 LEU B 81 -12.405 34.520 14.427	1.00 0.00 H 1.00 0.00 H 1.00 0.00 H 1.00 0.00 H
ATOM 3996 2HD1 LEU B 81 -13.691 35.135 13.359 ATOM 3997 3HD1 LEU B 81 -13.915 33.631 14.207 ATOM 3998 1HD2 LEU B 81 -11.952 31.695 13.726	1.00 0.00 H 1.00 0.00 H 1.00 0.00 H
ATOM 4000 3HD2 LEU B 81 -12.001 31.377 11.982 ATOM 4001 N GLU B 82 -10.987 36.068 11.529 ATOM 4002 CA GLU B 82 -0.987 36.068 11.529	1.00 0.00 H 1.00 0.00 H 1.00 0.09 N
ATOM 4003 C GLU B 82 -8.969 35.717 12.660 1 ATOM 4004 O GLU B 82 -9.443 35.926 13.776 1 ATOM 4005 CB GLU B 82 -9.250 37.831 11.486 1	1.00 0.09 C 1.00 0.09 C 1.00 0.09 O 1.00 0.09 C
ATOM 4006 CG GLU B 82 -9.774 38.615 10.282 1 ATOM 4007 CD GLU B 82 -9.587 40.099 10.568 1 ATOM 4008 OE1 GLU B 82 -9.587 40.458 11.201 1	1.00 0.09 C 1.00 0.09 C 1.00 0.09 O
35 ATOM 4010 H GLU B 82 -11.437 36.370 12.385 1 ATOM 4011 HA GLU B 82 -9.165 35.902 10.521 1 ATOM 4012 1HB GLU B 82 -8.149 37.899 11.523 1	1.00 0.09 01- 1.00 0.00 H 1.00 0.00 H 1.00 0.00 H
ATOM 4014 1HG GLU B 82 -9.643 38.266 12.420 1 ATOM 4014 1HG GLU B 82 -10.829 38.415 10.073 1 ATOM 4015 2HG GLU B 82 -9.148 38.392 9.408 1	1.00 0.00 H 1.00 0.00 H 1.00 0.00 H
ATOM 4017 CA VAL B 83 -7.263 34.328 13.611 1 ATOM 4018 C VAL B 83 -5.290 34.938 13.711 1 ATOM 4019 O VAL B 83 -5.239 35.146 12.700 1	L.00 0.09 N L.00 0.09 C L.00 0.09 C
45 ATOM 4021 CB VAL B 83 -7.069 32.850 13.470 1. ATOM 4021 CG1 VAL B 83 -8.451 32.182 13.377 1. ATOM 4022 CG2 VAL B 83 -6.170 32.598 12.250 1.	.00 0.09 C
ATOM 4024 HA VAL B 83 -7.846 34.520 14.521 1. ATOM 4025 HB VAL B 83 -6.558 32.481 14.379 1.	.00 0.00 н .00 0.00 н
ATOM 4027 2HG1 VAL B 83 -9.129 32.558 14.160 1. ATOM 4028 3HG1 VAL B 83 -8.933 32.369 12.403 1. ATOM 4029 1HG2 VAL B 83 -6.508 31.805 11.601 1.	.00 0.00 H .00 0.00 H .00 0.00 H
55 ATOM 4030 2HG2 VAL B 83 -6.129 33.419 11.520 1. ATOM 4031 3HG2 VAL B 83 -5.180 32.524 12.716 1. ATOM 4032 N PHE B 84 -5.469 35.260 14.943 1.	.00 0.00 H .00 0.00 H .00 0.23 N
ATOM 4034 C PHE B 84 -3.459 35.119 16.138 1. ATOM 4035 O PHE B 84 -4.077 34.442 16.959 1.	.00 0.23 C .00 0.23 C
ATOM 4037 CG PHE B 84 -5.215 38.093 14.810 1.0 ATOM 4038 CD1 PHE B 84 -4.889 38.632 13.590 1.0 ATOM 4039 CD2 PHE B 84 -6.487 38.271 15.293 1.0	00 0.23 C
65 ATOM 4041 CE2 PHE B 84 -5.814 39.344 12.865 1.0 ATOM 4042 CZ PHE B 84 -7.414 38.983 14.572 1.0 ATOM 4043 H PHE B 84 -7.081 39.525 13.357 1.0	00 0.23 C 00 0.23 C 00 0.23 C
70 ATOM 4043 H PHE B 84 -6.045 35.205 15.777 1.0 ATOM 4044 HA PHE B 84 -3.619 35.831 14.132 1.0 ATOM 4045 1HB PHE B 84 -3.221 37.757 15.548 1.0 ATOM 4046 2HB PHE B 84 -4.503 37.318 16.673 1.0 ATOM 4047 HD1 PHE B 84 -3.881 38.507 13.203 1.0	00 0.00 H 00 0.00 H 00 0.00 H

	ATO ATO	M 4049 H	ID2 PHE B IE1 PHE B IE2 PHE B	84 -6.1 84 -5.5 84 -8.4	32 39.80	0 11.919	1.00 0.	00 н
5	ATO ATO ATO	M 4051 H M 4052 N M 4053 C	Z PHE B SER B A SER B	84 -7.7 85 -2.1 85 -1.3	738 40.27 115 35.18 195 34.57	8 13.011 7 16.131 4 17.204	1.00 0.0	00 H 34 N
10	ATOM ATOM ATOM ATOM	4 4055 O 4 4056 C 4 4057 O	SER B B SER B	85 -0.6 85 0.3 85 -0.3 85 0.6	88 36.12 70 33.520	6 17.488 0 16.748	1.00 0.3 1.00 0.3 1.00 0.3	34 C 34 C
	ATOM ATOM ATOM	1 4059 H	A SER B B SER B	85 -1.5 85 -2.0 85 -0.8 85 0.1	92 35.821 77 34.071 58 32.718	15.547 17.905 16.180	1.00 0.0 1.00 0.0 1.00 0.0	00 н 00 н
15	ATOM ATOM ATOM ATOM	4062 HG 4063 N 4064 CA	SER B ASP B ASP B	85 0.8 86 -1.2 86 -0.6	96 34.924 55 36.148 46 37.204	16.364 19.032 19.785	1.00 0.0 1.00 0.0 1.00 0.2 1.00 0.2	0 H
20	ATOM ATOM ATOM	4066 O 4067 CE 4068 CG		86 -0.99 86 -1.89 86 -1.20 86 -0.79	50 36.156 09 38.597	21.535 19.458	1.00 0.2 1.00 0.2 1.00 0.2	3 C 3 O 3 C
25	MOTA MOTA MOTA MOTA	4070 OD	1 ASP B 2 ASP B ASP B	86 0.43 86 -1.58 86 -2.09 86 0.45	36 38.705 31 39.538 38 35.791	17.730 17.294 19.438	1.00 0.23 1.00 0.23 1.00 0.00	3 0 3 01-
	ATOM ATOM ATOM ATOM	4073 1HB 4074 2HB 4075 N	ASP B ASP B TRP B	86 -0.72 86 -2.26 87 -0.19	39.310 38.846 9 37.567	19.655 20.149 19.445 22.136	1.00 0.00 1.00 0.00 1.00 0.10) н
30	ATOM ATOM ATOM	4076 CA 4077 C 4078 O 4079 CB	TRP B	87 -0.48 87 -1.78 87 -2.58 87 0.60	2 37.995 7 37.390	23.524 23.895 24.598 24.479	1.00 0.14 1.00 0.14 1.00 0.14	C C C
35	ATOM ATOM ATOM ATOM	4082 CD	TRP B (87 1.76 87 3.02 87 1.66	0 36.923 5 36.993 0 35.660	24.577 24.074 25.254	1.00 0.14 1.00 0.14 1.00 0.14 1.00 0.14	C
40	ATOM ATOM ATOM	4084 CE2 4085 CE3 4086 CZ2	TRP B 6	3.72 37 2.89 37 0.62 37 3.10	2 35.022 1 35.080	24.401 25.126 25.924 25.670	1.00 0.14 1.00 0.14 1.00 0.14 1.00 0.14	
40	ATOM ATOM ATOM ATOM	4087 CZ3 4088 CH2 4089 H 4090 HA	TRP B 8	37 0.839 37 2.058 37 0.548 37 -0.614	33.837 33.201 38.189	26.474 26.350 21.872	1.00 0.14 1.00 0.14 1.00 0.00	C H
45	ATOM ATOM ATOM	4091 1HB 4092 2HB 4093 HD1	TRP B 8 TRP B 8 TRP B 8	7 0.152 7 0.938 7 3.478	37.992 38.892 37.795	24.197	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	H H H H
50	ATOM ATOM ATOM ATOM	4095 HE3 4096 HZ2	TRP B 8 TRP B 8 TRP B 8	7 -0.335 7 4.0 70	35.580 33.292	26.045 25.578	1.00 0.00 1.00 0.00 1.00 0.00 1.00 0.00	H H H
	ATOM ATOM ATOM ATOM	4098 HH2 4099 N 4100 CA 4101 C	TRP B 81 LEU B 81 LEU B 81	7 2.209 8 -2.035 8 -3.244	32.237 39.229 39.894	26.826 23.423 23.818	1.00 0.00 1.00 0.12 1.00 0.12	H H N C
55	MOTA MOTA MOTA	4102 O 4103 CB 4104 CG	LEU B 88 LEU B 88	9 -3.126 9 -2.988	40.527 40.978 41.028 41.777	21.717 1 24.827 1	1.00 0.12 1.00 0.12 1.00 0.12 1.00 0.12	0000
60	ATOM ATOM ATOM ATOM	4106 CD2 4107 H	LEU B 88 LEU B 88 LEU B 88	-3.893 -1.477	40.882 43.089 39.686	26.135 1 26.012 1 22.720 1	.00 0.12 .00 0.12 .00 0.00	C H
65	MOTA MOTA MOTA MOTA	4109 1HB 4110 2HB 4111 HG	LEU B 88 LEU B 88 LEU B 88	-2.285 -2.468 -4.825	41.747 40.616 42.096	2 4. 367 1 25.711 1	.00 0.00 .00 0.00 .00 0.00	H H H H
	ATOM ATOM ATOM	4112 1HD1 4113 2HD1 4114 3HD1 4115 1HD2	LEU B 88 LEU B 88	-4.833 -5.149	40.971 39.841 41.201	25.827 1 26.171 1 27.192 1	.00 0.00 .00 0.00 .00 0.00	H H H
70	ATOM ATOM ATOM	4116 2HD2 : 4117 3HD2 :	LEU B 88		42.897 2 43.720 2	26.951 1 25.387 1	.00 0.00 .00 0.00 .00 0.00 .00 0.11	H H H N

5	ATOM ATOM ATOM ATOM	4 4120 4 4121 4 4122	C LET CB LET	JB 8 JB 8 JB 8	9 -5.8 9 -7.0 9 -7.6 9 -6.3	20 41.926 08 41.536	21.934 22.942	1.00	0.11 0.11 0.11 0.11	C C O C
	ATON ATON ATON ATON ATON	4124 4125 4126	CG LET CD1 LET CD2 LET H LEU HA LEU	JB 8 JB 8 JB 8	9 -6.00 9 -7.71 9 -5.79	01 41.822 12 39.917 91 40.201	19.129 18.356 18.228 23.266	1.00 1.00 1.00 1.00	0.11 0.11 0.11 0.00	н С С
10	ATOM ATOM ATOM ATOM	4128 4129 4130 4131	1HB LEU 2HB LEU HG LEU 1HD1 LEU	B 89	9 -7.01 9 -5.45 9 -7.82	39.506 39.693 8 41.548	20.758	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
15	MOTA MOTA MOTA MOTA MOTA	4133 4134 4135	2HD1 LEU 3HD1 LEU 1HD2 LEU 2HD2 LEU 3HD2 LEU	B 89 B 89	-5.12 -8.14 -7.00	6 41.235 2 40.512 7 39.183	18.958 18.030 17.418 17.817	1.00 1.00 1.00 1.00	0.00 0.00 0.00	н н н н
20	ATOM ATOM ATOM ATOM	4137 4138 4139 4140	N LEU CA LEU C LEU O LEU	B 90 B 90 B 90	-7.40 -8.59 -9.60	0 43.026 7 43.700 6 43.186	18.761 21.259 21.649 20.677 19.467	1.00 1.00 1.00 1.00	0.00 0.11 0.11 0.11	H N C C
25	MOTA MOTA MOTA MOTA MOTA	4141 4142 4143 4144 4145	CB LEU CG LEU CD1 LEU CD2 LEU H LEU	B 90 B 90 B 90	-8.52 -9.810 -10.083 -9.793 -6.910	8 45.948 3 45.729 3 47.437	21.510 21.950 23.448 21.568	1.00 1.00 1.00 1.00	0.11 0.11 0.11 0.11	0000
30	MOTA MOTA MOTA MOTA MOTA	4146 4147 1 4148 2 4149	HA LEU	B 90 B 90 B 90 B 90	-8.843 -8.289 -7.683 -10.652	3 43.446 9 45.492 8 45.608 45.497	20.450 22.688 20.463 22.117 21.379		0.00 0.00 0.00 0.00	н н н н
35	MOTA ATOM ATOM ATOM	4151 2 4152 3 4153 1 4154 2	HD1 LEU HD1 LEU HD2 LEU HD2 LEU	B 90 B 90 B 90	-11.099 -9.407 -9.921 -10.779 -9.068	44.997 46.663 47.894 47.981	23.615 23.914 24.002 21.677 22.192	1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H H
40	ATOM ATOM ATOM ATOM ATOM	4156 1 4157 (4158 (HD2 LEU N GLN CA GLN C GLN C GLN	B 91 B 91 B 91	-9.494 -10.719 -11.640 -12.857 -13.277	42.628 41.998 42.848	20.513 21.185 20.289 20.152 21.093	1.00 1.00 1.00 1.00	0.00 0.11 0.11 0.11	H N C C
45	ATOM ATOM ATOM ATOM	4161 (4162 (4163 (CB GLN I CG GLN I CD GLN I DE1 GLN I	B 91 B 91 B 91 B 91	-12.096 -10.956 -11.531 -12.410	40.612 39.593 38.284 38.286	20.782 20.886 21.415 22.275	1.00 (1.00 (1.00 (0.11 0.11 0.11 0.11	0 0 0 0
50	ATOM ATOM ATOM ATOM ATOM	4165 H	A GLN I	91 91 91	-11.026 -10.874 -11.163 -12.816 -12.614		19.308 20.042	1.00 0 1.00 0 1.00 0	0.11 0.00 0.00 0.00	N H H H
e e	ATOM ATOM ATOM ATOM	4169 1H 4170 2H 4171 1H 4172 2H	G GLN E	91 91 91	-10.184 -10.464 -10.465 -11.449	39.916 39.476 37.207	21.606 19.910 20.058	1.00 0 1.00 0 1.00 0	.00	H H H
55	ATOM ATOM ATOM ATOM ATOM	4173 N 4174 C 4175 C 4176 O	A ALA B ALA B ALA B	92 92 92	-13.435 -14.630 -15.533 -15.082	42.855 43.605 42.758 41.941	18.936 18.701 17.870	1.00 0 1.00 0 1.00 0	.18 .18 .18	H C C
60	ATOM ATOM ATOM ATOM	4177 CT 4178 H 4179 HZ 4180 1HI 4181 2HI	ALA B ALA B B ALA B		-14.397 -13.113 -15.098 -15.350 -13.693	42.309 3 43.889 3 45.450 1	18.152 1 19.650 1 17.815 1	1.00 0 1.00 0 1.00 0	.18 .00 .00 .00	C H H H
65	ATOM ATOM ATOM ATOM	4182 3HE 4183 N 4184 CA 4185 C	S ALA B SER B SER B SER B	92 93 93	-13.093 -13.990 -16.852 -17.796 -17.756	44.720 1 42.907 1 42.156 1	6.918 1 8.076 1 7.309 1	.00 0.	.00 .00 .25 .25	H N C C
70	ATOM ATOM ATOM ATOM	4186 O 4187 CB 4188 OG 4189 H		93 93 93	-17.703 -19.230 -20.123 -17.207	41.842 1 42.324 1 41.558 1	4.957 1 7.826 1 7.034 1	.00 0. .00 0.	25 25 25	о с о н

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4190 4191 4192 4193 4194 4195 4196 4197	HA 1HB 2HB HG N CA C	SER SER SER SER ALA ALA ALA	B 9. B 9. B 9. B 9. B 9.	3 -19.54; 3 -19.31; 3 -20.01; 4 -17.76; 4 -17.77; 4 -16.91;	2 43.384 4 41.932 1 41.846 9 43.973 7 44.482 9 45.705	17.844 18.849 16.114 15.694 14.351 14.290	1.00 1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.19 0.19 0.19	H H H N C
10	MOTA MOTA MOTA MOTA	4198 4199 4200 4201	CB H HA 1HB	ALA ALA ALA	B 94 B 94 B 94	4 -19.179 4 -17.658 4 -17.356 4 -19.117	44.880 44.650 43.726 45.246	13.860 16.428 13.667 12.823	1.00 1.00 1.00 1.00	0.19 0.19 0.00 0.00	О Н Н Н
15	MOTA MOTA MOTA MOTA MOTA	4203 4204 4205 4206	2HB 3HB N CA C	ALA GLU GLU GLU	B 95 B 95 B 95	4 -19.612 5 -16.301 5 -15.454	45.677 45.923 47.050	13.878 14.484 13.114 12.861 12.802	1.00 1.00 1.00	0.00 0.00 0.12 0.12 0.12	н и с с
20	MOTA MOTA MOTA MOTA MOTA	4207 4208 4209 4210 4211	O CB CG CD OE1	GLU GLU GLU GLU	B 95 B 95 B 95	5 -14.711 5 -13.753 5 -13.312	46.900 45.702 45.440	13.378 11.522 11.506 10.073 9.208	1.00 1.00 1.00 1.00	0.12 0.12 0.12 0.12	0000
25	ATOM ATOM ATOM ATOM ATOM	4212 4213 4214 4215 4216 2	OE2 H HA LHB	GTN GTN GTN	B 95 B 95 B 95 B 95	-12.742 -16.316 -14.722 -14.146	44.344 45.238 47.164 47.836	9.826 12.374 13.677 11.359	1.00 1.00 1.00 1.00	0.12 0.12 0.00 0.00 0.00	0 01- H H H
30	MOTA MOTA MOTA MOTA	4217 1 4218 2 4219 4220	HG HG N CA	GLU GLU GLU VAL VAL	B 95 B 95 B 96 B 96	-14.200 -12.869 -17.436 -18.234	44.777 45.899	10.703 11.906 12.134 12.110 11.956	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.11 0.11	H H N C
35	ATOM ATOM ATOM ATOM ATOM			VAL I VAL I VAL I VAL I	B 96 B 96 B 96	-20.025 -18.599 -19.514 -17.299	49.229 48.119 49.704 50.942 49.864	12.709 12.813 10.531 10.495 9.726	1.00 1.00 1.00 1.00	0.11 0.11 0.11 0.11 0.11	0 0 0 0
40	ATOM ATOM ATOM ATOM ATOM	4227 4228		VAL II VAL II VAL II VAL II	96 3 96 3 96	-17.804 -17.676	47.378 50.279 48.857 51.278 50.663	11.744 12.332 10.104 9.448 10.851	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H H
45	ATOM ATOM ATOM ATOM ATOM	4231 3 4232 1 4233 2 4234 3	HG1 HG2 HG2 HG2	VAL E VAL E VAL E	96 96 96 96 96	-19.099 -17.491 -16.616 -16.754	51.777 50.218 50.584 48.909	11.077 8.699 10.198 9.632	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
50	ATOM ATOM ATOM ATOM	4236 4237 4238	CA C O	VAL E VAL E VAL E VAL B	97 97 97	-20.028 -21.230 -22.100 -21.654 -20.992	50.335 50.266 51.399 52.332 50.434	13.268 14.039 13.620 12.957 15.511	1.00 1.00 1.00 1.00	0.10 0.10 0.10 0.10 0.10	N C O C
55	MOTA MOTA MOTA MOTA	4241 (4242 1 4243 1	CG2 H HA	VAL B VAL B VAL B VAL B VAL B	97 97 97	-20.128 -20.363 -19.530 -21.758 -21.926	49.263 51.816 51.212 49.333	16.004 15.752 13.277 13.789	1.00 1.00 1.00 1.00	0.10 0.10 0.00 0.00	С Н Н
60	ATOM ATOM ATOM ATOM	4245 11 4246 21 4247 31 4248 11	HG1 HG1 HG1 HG2	VAL B VAL B VAL B VAL B	97 97 97 97	-20.116 -20.458 -19.079 -20.214	50.484 49.203 48.283 49.385 51.976	16.060 17.104 15.626 15.681 16.835	1.00 1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H H
	ATOM ATOM ATOM ATOM ATOM	4249 2F 4250 3F 4251 N 4252 0 4253 0	ig2 v V i CA i		97 97 98 98 98	-19.366 -21.003 -23.386 -24.315 -24.355	51.909 52.645 51.330 52.369 53.226	15.298 15.413 14.004 13.688 14.909	1.00 1.00 1.00 1.00	0.00 0.00 0.12 0.12 0.12	H N C C
65	MOTA MOTA MOTA MOTA	4254 C 4255 C 4256 C 4257 S	B N G N	CET B CET B CET B CET B	98 98 98 98	-24.093 -25.737 -25.810 -25.466	52.749 51.837 50.833 51.524	16.012 13.442 12.286 10.639	1.00 1.00 1.00 1.00	0.12 0.12 0.12 0.12	0 C C s
70	ATOM ATOM ATOM	4259 H	I M	CET B CET B	98 98 98	-27.170 -23.734 -24.011	52.062 50.567 52.927	10.325 14.559 12.813	1.00	0.12 0.00 0.00	C H H

	MOTA MOTA MOTA	4261 1HE 4262 2HE 4263 1HG	MET B 98	-26.107	52.694 51.339 50.356	14.356	1.00	0.00 0.00 0.00	H H H
5	MOTA MOTA MOTA	4264 2HG 4265 1HE 4266 2HE	MET B 98 MET B 98	-27.192	50.010 52.555 51.201			0.00 0.00 0.00	н н н
10	ATOM ATOM ATOM	4267 3HE 4268 N 4269 CA	GLU B 99 GLU B 99	-24.653 -24.662	52.785 54.527 55.336	11.086 14.755 15.936	1.00 1.00 1.00	0.00 0.10 0.10	H N C
10	MOTA MOTA MOTA MOTA	4270 C 4271 O 4272 CB 4273 CG		-26.866 -24.838	54.890 54.525 56.844 57.670	16.779 16.272 15.682 16.970	1.00 1.00 1.00 1.00	0.10 0.10 0.10 0.10	0 0 0
15	ATOM ATOM	4274 CD 4275 OE		-24.956 -24.323	59.140 59.619 59.803	16.629 15.652 17.347	1.00 1.00 1.00	0.10 0.10 0.10	c 0 01-
20	ATOM ATOM ATOM	4277 H 4278 HA 4279 1HB	GLU B 99	-23.696 -25.788	54.937 55.198 57.005	13.900 16.459 15.155	1.00 1.00 1.00	0.00	н н н
20	ATOM ATOM ATOM ATOM	4280 2HB 4281 1HG 4282 2HG 4283 N	GLU B 99 GLU B 99 GLU B 100	-23.975 -23.715 -25.443 -25.599	57.166 57.578 57.385 54.893	15.117 17.265 17.776 18.108	1.00 1.00 1.00	0.00 0.00 0.00 0.20	H H H N
25	MOTA MOTA MOTA	4284 CA 4285 C 4286 O	GLY B 100 GLY B 100 GLY B 100	-26.641 -26.474 -27.034	54.528 53.096 52.656	19.014 19.396 20.399	1.00 1.00 1.00	0.20 0.20 0.20	c c o
30	MOTA MOTA MOTA MOTA	4287 H 4288 1HA 4289 2HA 4290 N	GLY B 100 GLY B 100 GLY B 100 GLN B 101	-24.793 -27.635 -26.586 -25.696	55.390 54.668 55.155 52.315	18.492 18.562 19.915 18.624	1.00 1.00 1.00	0.00 0.00 0.00 0.50	H H H
	MOTA MOTA MOTA	4291 CA 4292 C 4293 O	GLN B 101 GLN B 101 GLN B 101	-25.580 -24.520 -23.614	50.950 50.860 51.689	19.038 20.078 20.161	1.00 1.00 1.00	0.50 0.50 0.50	И С С О
35	MOTA MOTA MOTA	4294 CB 4295 CG 4296 CD	GLN B 101 GLN B 101 GLN B 101	-25.311 -23.985 -23.925	49.923 50.050 48.857	17.920 17.175 16.224	1.00 1.00 1.00	0.50 0.50 0.50	с с с
40	ATOM ATOM ATOM ATOM	4297 OE2 4298 NE2 4299 H 4300 HA	GLN B 101 GLN B 101 GLN B 101 GLN B 101	-22.862 -25.114 -25.185 -26.589	48.448 48.265 52.658 50.647	15.763 15.932 17.818 19.360	1.00 1.00 1.00 1.00	0.50 0.50 0.00 0.00	O H H
	ATOM ATOM ATOM	4301 1HB 4302 2HB 4303 1HG	GLN B 101 GLN B 101 GLN B 101	-26.170 -25.362 -23.127	50.034 48.930 49.980	17.236 18.402 17.861	1.00 1.00 1.00	0.00 0.00 0.00	н н н
45	ATOM ATOM ATOM ATOM	4304 2HG 4305 1HE2 4306 2HE2 4307 N		-23.855 -25.978 -25.070 -24.671	50.850 48.551 47.437	16.515 16.350 15.362	1.00 1.00 1.00	0.00 0.00 0.00	H H H
50	ATOM ATOM ATOM	4308 CA 4309 C 4310 O	PRO B 102 PRO B 102 PRO B 102	-23.702 -22.464 -22.552	49.879 49.696 49.090 48.324	20.918 21.956 21.396 20.440	1.00 1.00 1.00	0.57 0.57 0.57 0.57	N C C
	ATOM ATOM ATOM ATOM	4311 CB 4312 CG 4313 CD 4314 HA	PRO B 102 PRO B 102 PRO B 102 PRO B 102	-24.375 -25.870 -26.007 -23.501	48.836 49.147 49.500 50.683	23.023 22.846 21.355 22.400	1.00 1.00 1.00 1.00	0.57 0.57 0.57 0.00	C C H
55	MOTA MOTA ATOM	4315 1HB 4316 2HB 4317 1HG	PRO B 102 PRO B 102 PRO B 102	-23.985 -24.196 -26.136	49.030 47.767 50.022	24.034 22.814 23.462	1.00 1.00 1.00	0.00 0.00 0.00	н н н
60	ATOM ATOM ATOM ATOM	4318 2HG 4319 1HD 4320 2HD 4321 N	PRO B 102 PRO B 102 PRO B 102 LEU B 103	-26.538 -26.352 -26.737 -21.299	48.328 48.634 50.310 49.426	23.154 20.768 21.257 21.973	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.26	H H H N
C.F.	ATOM ATOM ATOM	4322 CA 4323 C 4324 O	LEU B 103 LEU B 103 LEU B 103	-20.081 -19.597 -19.568	48.841 47.982 48.404	21.517 22.628 23.782	1.00 1.00 1.00	0.26 0.26 0.26	с с о
65	ATOM ATOM ATOM ATOM		LEU B 103 LEU B 103 LEU B 103 LEU B 103	-18.971 -17.661 -17.856 -16.509	49.863 49.217 48.516 50.235	21.213 20.720 19.366 20.709	1.00 1.00 1.00 1.00	0.26 0.26 0.26 0.26	0000
70	ATOM ATOM ATOM	4329 H 4330 HA 4331 1HB	LEU B 103 LEU B 103 LEU B 103	-21.251 -20.277 -18.745	50.111 48.257 50.421	20.709 22.718 20.607 22.129	1.00 1.00 1.00	0.00 0.00 0.00	H H H

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4334 1: 4335 2: 4336 3: 4337 1: 4338 2:	HB LEU HG LEU HD1 LEU HD1 LEU HD1 LEU HD2 LEU HD2 LEU HD2 LEU HD2 LEU	B 103 B 103 B 103 B 103 B 103	-17.359 -16.913 -18.596 -18.182 -15.604 -16.779	48.441 48.068 47.704 49.236 49.827 51.152	21.447 19.010 19.406 18.598 20.237 20.160	1.00 1.00 1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00 0.00	н н н н н
10	MOTA MOTA MOTA MOTA	4340 1 4341 0 4342 0 4343 0	PHE PHE PHE PHE	B 104 B 104 B 104 B 104	-19.234 -18.730 -17.343 -17.099	46.729 45.879 45.523 45.161	22.312 23.344 22.936 21.785	1.00 1.00 1.00 1.00	0.08 0.08 0.08	н С С О
15	MOTA MOTA MOTA MOTA MOTA	4345 0 4346 0 4347 0 4348 0		B 104		43.851 44.202		1.00 1.00 1.00	0.08 0.08 0.08 0.08	00000
20	ATOM ATOM ATOM ATOM ATOM	4350 C 4351 H	PHE A	B 104 B 104 B 104 B 104 B 104	-17.597 -17.990 -19.164 -18.730 -19.479	42.141 42.502 46.378 46.402 43.969	25.630 26.896 21.373 24.309 22.596	1.00 1.00 1.00 1.00	0.08 0.00 0.00	С Н Н
25	ATOM ATOM ATOM ATOM ATOM	4354 2H 4355 H 4356 H 4357 H	B PHE 1 D1 PHE 1 D2 PHE 1 E1 PHE 1	B 104 B 104 B 104 B 104	-20.591 -20.096 -18.020 -19.224	44.822 45.005 42.448 43.802	23.665 26.104 23.527 28.062	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H H
30	MOTA MOTA MOTA MOTA	4359 H 4360 N 4361 C 4362 C	LEU I A LEU I LEU I	B 104 B 105 B 105 B 105	-16.936 -17.766 -16.385 -15.028 -14.558	41.303 41.863 45.650 45.325 44.396	25.591 27.735 23.872 23.562 24.624	1.00 1.00 1.00 1.00	0.00 0.00 0.10 0.10 0.10	H N C C
35	MOTA MOTA MOTA MOTA MOTA		B LEU F	3 105 3 105 3 105	-15.108 -14.079 -14.388 -13.388 -14.485	44.362 46.536 47.582 48.748 46.936	25.724 23.569 22.481 22.534 21.090	1.00 1.00 1.00 1.00	0.10 0.10 0.10 0.10 0.10	00000
40	ATOM ATOM ATOM ATOM ATOM	4368 H 4369 H 4370 1H 4371 2H	LEU E LEU E LEU E LEU E	3 105 3 105 3 105 3 105	-16.576 -14.968 -13.123 -13.791	45.939 44.805 46.086 46.969	24.827 22.597 23.234 24.481	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
4 5	ATOM ATOM ATOM ATOM	4372 He 4373 1Hi 4374 2Hi 4375 3Hi 4376 1Hi)1 LEU B)1 LEU B	105 105 105	-15.382 -13.415 -13.615 -12.365 -14.787	48.018 49.365 49.414 48.392 47.681	22.698 21.621 23.383 22.683 20.341	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H H
50	ATOM ATOM ATOM	4377 2HI 4378 3HI 4379 N 4380 C	2 LEU B 2 LEU B ARG B . ARG B	105 105 106 106	-13.499 -15.189 -13.530 -13.059	46.550 46.111 43.592 42.656	20.781 20.996 24.307 25.276	1.00 1.00 1.00 1.00	0.00 0.00 0.15 0.15	H H N C
	MOTA MOTA MOTA MOTA MOTA MOTA	4381 C 4382 O 4383 CE 4384 CG 4385 CD	ARG B	106 106 106	-11.579 -11.049 -13.663 -13.241 -14.061	42.563 42.581 41.262 40.162 38.888	25.130 24.020 25.034 26.004	1.00	0.15	0000
55	MOTA MOTA MOTA MOTA	4386 NE 4387 CZ 4388 NH 4389 NH	ARG B ARG B 1 ARG B 2 ARG B	106 106 106 106	-13.541 -12.993 -12.935 -12.531	37.832 36.702 36.556 35.718	25.787 26.698 26.169 24.813 26.995	1.00 1.00 1.00 1.00	0.15 0.15 0.15 0.15 0.15	C N1+ C N N
60	ATOM ATOM ATOM ATOM ATOM	4390 H 4391 HA 4392 1HB 4393 2HB 4394 1HG	ARG B ARG B ARG B ARG B ARG B	106 106 106	-13.089 -13.331 -13.453 -14.740	43.585 42.978 40.935 41.426	23.398 26.288 24.002 25.150	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н
65	MOTA MOTA MOTA	4395 2HG 4396 1HD 4397 2HD 4398 HE	ARG B ARG B ARG B	106 106 106 106	-13.146 -12.200 -13.950 -15.136 -13.935	40.446 39.888 38.632 39.011 37.715	27.059 25.736 24.738 25.994 27.606		0.00 0.00 0.00 0.00	н н н н
70	ATOM ATOM ATOM ATOM	4399 1HH 4400 2HH 4401 1HH 4402 2HH	ARG B	106 106		34.859	24.200 24.442 26.638 27.979	1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H

	ATOM ATOM	4403 4404	n ca	CYS CYS		107 107	-10.862 -9.446	42.482 42.306	26.266 26.188	1.00	0.16 0.16	N C
	ATOM	4405	C	CYS		107	-9.261	40.846	26.416	1.00	0.16	C
_	MOTA	4406	0	CYS		107	-9.650	40.320	27.458	1.00	0.16	0
5	MOTA	4407	CB	CYS			-8.663	43.074	27.268	1.00	0.16	C
	MOTA	4408	SG	CYS		107	-9.006	44.857	27.207	1.00	0.16 0.00	S H
	ATOM ATOM	4409 4410	H HA	CYS		107	-11.264 -9.062	42.454 42.647	27.191 25.214	1.00 1.00	0.00	H
	MOTA	4411	1HB	CYS		107	-7.591	42.892	27.084	1.00	0.00	н
10	ATOM	4412	2HB	CYS			-8.887	42.711	28.282	1.00	0.00	H
	MOTA	4413	N	HIS		108	-8.681	40.141	25.429	1.00	0.11	N
	MOTA	4414	CA	HIS		108	-8.593	38.719	25.557	1.00	0.11	C
	MOTA	4415	c	HIS HIS		108	-7.159	38.316	25.545	1.00	0.11	С 0
15	ATOM ATOM	4416 4417	O CB	HIS		108	-6.360 -9.321	38.829 37.991	24.763 24.412	1.00 1.00	0.11	c
10	ATOM	4418	CG	HIS		108	-9.314	36.494	24.517	1.00	0.11	Č
	ATOM	4419		HIS		108	-8.352	35.693	23.946	1.00	0.11	N
	MOTA	4420		HIS		108	-10.189	35.649	25.126	1.00	0.11	С
•	MOTA	4421		HIS		108	-8.693	34.410	24.231	1.00	0.11	C
20	ATOM	4422		HIS		108	-9.799 -8.343	34.333 40.550	24.946 24.563	1.00 1.00	0.11	N H
	ATOM ATOM	4423 4424	H HA	HIS HIS		108	-9.067	38.390	26.494	1.00	0.00	H
	MOTA	4425		HIS		108	-8.903	38.313	23.443	1.00	0.00	н
	ATOM	4426		HIS		108	-10.372	38.319	24.407	1.00	0.00	H
25	MOTA	4427		HIS		108	-10.626	35.988	26.029	1.00	0.00	H
	MOTA	4428		HIS			-7.908	33.691	24.152	1.00	0.00	H
	ATOM	4429		HIS GLY		108	-9.908 -6.805	33.580 37.367	25.609 26.433	1.00 1.00	0.00 0.09	H N
	ATOM ATOM	4430 4431	N CA	GLY			-5.456	36.899	26.515	1.00	0.09	Ċ
30	ATOM ATOM	4432	C	GLY			-5.417	35.556	25.871	1.00	0.09	Č
-	ATOM	4433	0	GLY			-6.414	34.837	25.839	1.00	0.09	0
	ATOM	4434	H	GLY			-7.478	36.848	26.971	1.00	0.00	H
	MOTA	4435	1HA	GLY			-5.161	36.786	27.574	1.00	0.00	H
35	ATOM	4436 4437	2HA N	GLY TRP			-4.766 -4.241	37.619 35.184	26.058 25.339	1.00 1.00	0.00	H N
33	ATOM ATOM	4438	CA	TRP			-4.097	33.932	24.665	1.00	0.32	Ĉ
	ATOM	4439	C .	TRP			-4.162	32.847	25.691	1.00	0.32	С
	MOTA	4440	0	TRP	В	110	-3.707	33.008	26.822	1.00	0.32	0
4.0	ATOM	4441	CB	TRP			-2.767	33.840	23.890	1.00	0.32	C
40	ATOM	4442 4443	CG	TRP TRP			-2.534 -3.146	32.551 32.070	23.142 22.021	1.00 1.00	0.32 0.32	C C
	ATOM ATOM	4444		TRP			-1.525	31.596	23.495	1.00	0.32	č
	ATOM	4445	NE1	TRP		110	-2.583	30.869	21.657	1.00	0.32	N
	MOTA	4446	CE2	TRP	В	110	-1.580	30.568	22.553	1.00	0.32	С
45	MOTA	4447	CE3	TRP			-0.621	31.578	24.517	1.00	0.32	C
	ATOM	4448		TRP			-0.729	29.502	22.620 24.583	1.00 1.00	0.32 0.32	C
	ATOM ATOM	4449 4450	CZ3 CH2	TRP		110	0.236 0.183	30.504 29.486	23.653	1.00	0.32	č
	ATOM	4451	H	TRP			-3.501	35.873	25.213	1.00	0.00	H
50	ATOM	4452	HA	TRP			-4.922	33.828	23.933	1.00	0.00	H
	ATOM	4453	1HB	TRP	В	110	-1.929	34.040	24.572	1.00	0.00	H
	MOTA	4454		TRP				34.667				H
	MOTA	4455		TRP			-4.013 -3.077	32.458 30.217	21.524 21.085	1.00 1.00	0.00	H H
55	MOTA MOTA	4456 4457		TRP			-0.604	32.378	25.237	1.00	0.00	H
J J	ATOM	4458		TRP			-0.771	28.699	21.889	1.00	0.00	H
	ATOM	4459		TRP			1.037	30.521	25.317	1.00	0.00	H
	ATOM	4460		TRP			0.902	28.670	23.710	1.00	0.00	H
CO	ATOM	4461	N	ARG			-4.775	31.709	25.311	1.00	0.53	N
60	ATOM	4462	CA	ARG ARG			-4.933 -5.683	30.586 31.000	26.189 27.413	1.00 1.00	0.53 0.53	c c
	ATOM ATOM	4463 4464	С 0	ARG			-5.653	30.300	28.425	1.00	0.53	Õ
	ATOM	4465	СВ	ARG			-3.620	29.933	26.655	1.00	0.53	C
	ATOM	4466	CG	ARG			-3.020	28.970	25.633	1.00	0.53	С
65	MOTA	4467	CD	ARG			-2.053	27.949	26.245	1.00	0.53	C
	MOTA	4468	NE	ARG			-0.754	28.629	26.508	1.00	0.53	N1+
	ATOM	4469	CZ NEL1	ARG ARG			0.186 -0.095	28.032 26.849	27.299 27.921	1.00	0.53 0.53	C N
	MOTA MOTA	4470 4471		ARG			1.396	28.633	27.493	1.00	0.53	N
70	MOTA	4472	Н	ARG			-5.186	31.627	24.389	1.00	0.00	H
	MOTA	4473	HA	ARG			-5.583	29.848	25.683	1.00	0.00	H

	ATOM	4474	1172	ARG	R	111	-3.792	29.342	27.570	1.00	0.00	н
	ATOM		2HB	ARG		111	-2.899	30.707	26.910	1.00	0.00	H
	ATOM	4476		ARG			-2.557	29.498	24.791	1.00	0.00	Н
	ATOM		2HG	ARG			-3.855	28.394	25.192	1.00	0.00	н
5	ATOM		1HD	ARG			-1.871	27.088	25.580	1.00	0.00	H
	ATOM	4479	2HD	ARG	В	111	-2.462	27.574	27.198	1.00	0.00	H
	ATOM	4480	HE	ARG			-0.400	29.179	25.751	1.00	0.00	H
	ATOM	4481					-0.987	26.418	27.837	1.00	0.00	H
4.0	MOTA		2HH1			111	0.584	26.383	28.480	1.00	0.00	H
10	ATOM		1HH2				2.095	28.219	28.070	1.00	0.00	H
	MOTA		2HH2				1.585	29.543	27.140	1.00	0.00	H
	MOTA	4485	N	ASN			-6.402 -7.191	32.134 32.586	27.343	1.00 1.00	0.33 0.33	N C
	MOTA MOTA	4486 4487	CA C	ASN ASN			-6.360	32.626	28.452 29.693	1.00	0.33	č
15	ATOM	4488	o	ASN			-6.800	32.181	30.754	1.00	0.33	ŏ
10	MOTA	4489	CB	ASN			-8.409	31.688	28.734	1.00	0.33	č
	ATOM	4490	CG	ASN			-9.405	31.882	27.605	1.00	0.33	c
	ATOM	4491		ASN			-9.721	33.014	27.241	1.00	0.33	0
	MOTA	4492	ND2	ASN	В	112	-9.908	30.756	27.031	1.00	0.33	N
20	ATOM	4493	H	ASN	В	112	-6.362	32.724	26.520	1.00	0.00	H
	MOTA	4494	HА	ASN		112	-7.515	33.623	28.253	1.00	0.00	H
	ATOM	4495		ASN			-8.936	32.044	29.637	1.00	0.00	H
	MOTA		2HB	ASN		112	-8.129	30.637	28.898	1.00	0.00	H
0.5	ATOM		1HD2			112	-9.555	29.853	27.290	1.00	0.00	H
25	ATOM		2HD2				-10.398	30.864	26.155	1.00	0.00	H
	ATOM	4499	N	TRP			-5.133	33.171	29.612	1.00	0.13	N
	MOTA	4500	CA	TRP TRP			-4.351	33.236	30.808	1.00	0.13 0.13	C C
	MOTA	4501 4502	С 0	TRP		113	-4.945 -5.619	34.304 35.209	31.665 31.177	$1.00 \\ 1.00$	0.13	õ
30	MOTA ATOM	4502	CB	TRP		113	-2.864	33.550	30.572	1.00	0.13	c
50	ATOM	4504	CG	TRP			-2.109	32.435	29.884	1.00	0.13	č
	ATOM	4505		TRP		113	-1.666	32.352	28.595	1.00	0.13	č
	ATOM	4506	CD2	TRP			-1.737	31.203	30.524	1.00	0.13	С
	ATOM	4507		TRP			-1.030	31.149	28.395	1.00	0.13	N
35	ATOM	4508	CE2	TRP			-1.071	30.431	29.574	1.00	0.13	С
	ATOM	4509	CE3	TRP	В	113	-1.939	30.749	31.798	1.00	0.13	С
	MOTA	4510	CZ2	TRP	В	113	-0.593	29.190	29.891	1.00	0.13	С
	MOTA	4511	CZ3	TRP			-1.451	29.499	32.110	1.00	0.13	C
	ATOM	4512	CH2	TRP		113	-0.791	28.733	31.174	1.00	0.13	c
40	MOTA	4513	H	TRP		113	-4.706	33.392	28.722	1.00	0.00	H
	ATOM	4514	HA	TRP			-4.416	32.264	31.331	1.00	0.00	H
	ATOM	4515 4516	1HB	TRP		113	-2.398 -2.768	33.746 34. 49 0	31.554 30.007	1.00	0.00	H H
	ATOM ATOM	4517		TRP		113	-1.720	33.120	27.844	1.00	0.00	н
45	ATOM	4518		TRP			-0.986	30.689	27.511	1.00	0.00	H
10	ATOM	4519	HE3	TRP			-2.453	31.342	32.547	1.00	0.00	H
	ATOM	4520	HZ2	TRP		113	0.140	28.651	29.363	1.00	0.00	H
	ATOM	4521	HZ3	TRP	В	113	-1.587	29.113	33.118	1.00	0.00	H
	MOTA	4522	HH2	TRP	В	113	-0.388	27.770	31.480	1.00	0.00	H
50	MOTA	4523	N	ASP	В	114	-4.712	34.218	32.988	1.00	0.12	N
	MOTA	4524	CA	ASP			-5.293	35.164	33.895	1.00	0.12	C
	MOTA	4525	С	ASP			-4.813	36.522	33.513	1.00	0.12	C
	MOTA	4526	0	ASP			-3.627	36.729	33.263	1.00	0.12	0
	ATOM	4527	CB	ASP			-4.874	34.945	35.357	1.00	0.12	C
55	ATOM	4528	CG	ASP			-5.445	33.616	35.823	1.00	0.12	С 0
	ATOM	4529		ASP			-6.688 -4.640	33.434	35.731 36.285	1.00 1.00	0.12 0.12	01-
	ATOM	4530 4531	H	ASP ASP			-4.235	32.765 33.453	33.434	1.00	0.00	н
	MOTA	4532	HA	ASP			-6.396	35.103	33.822	1.00	0.00	н
60	MOTA MOTA		1HB	ASP			-5.326	35.762	35.943	1.00	0.00	H
00	ATOM	4534		ASP			-3.782	34.988	35.482	1.00	0.00	H
	ATOM	4535	N	VAL			-5.746	37.488	33.447	1.00	0.21	N
	ATOM	4536	CA	VAL			-5.368	38.823	33.098	1.00	0.21	c
	ATOM	4537	C	VAL			-5.975	39.733	34.112	1.00	0.21	Ċ
65	ATOM	4538	ō	VAL			-7.072	39.488	34.611	1.00	0.21	0
	ATOM	4539		VAL			-5.880	39.263	31.759	1.00	0.21	С
	MOTA	4540	CG1	VAL	В	115	-5.413	40.708	31.508	1.00	0.21	С
	MOTA	4541		VAL			-5.402	38.262	30.694	1.00	0.21	С
	MOTA	4542	H	VAL			-6.699	37.343	33.725	1.00	0.00	H
70	MOTA	4543		VAL			-4.271	38.918	33.117	1.00	0.00	H
	MOTA	4544	HB	VAL	В	115	-6.981	39.270	31.744	1.00	0.00	H

	ATOM	4545 1	HG1 V	L E	3 115	-5.622	41.014	30.468	1.00	0.00	Н
	MOTA	4546 2	HG1 V	L E	3 115	-5.940	41.434	32.142	1.00	0.00	H
	MOTA		HG1 V			-4.326	40.819	31.656	1.00	0.00	H
5	ATOM		HG2 V			-6.242	37.632	30.360 29.788	1.00	0.00	H
3	ATOM ATOM	4549 21 4550 31	HG2 V/			-5.022 -4.626	38.760 37.571	31.037	1.00	0.00	H H
	ATOM				3 116	-5.249	40.808	34.455	1.00	0.44	N
	ATOM				116	-5.738	41.756	35.407	1.00	0.44	С
	ATOM	4553			3 116	-5.192	43.082	34.997	1.00	0.44	С
10	ATOM				116	-4.387	43.164	34.070	1.00	0.44	0
	ATOM				3 116	-5.271	41.458	36.836	1.00	0.44	C
	ATOM ATOM		CG TY		116	-3.794 -2.990	41.347	36.746 36.891	1.00	0.44	C C
	ATOM		CD2 TY			-3.215	40.131	36.486	1.00	0.44	c
15	MOTA		CE1 TY			-1.624	42.331	36.797	1.00	0.44	č
	ATOM	4560	CE2 TY	R E	116	-1.851	40.007	36.391	1.00	0.44	С
	ATOM				116	-1.050	41.109	36.548	1.00	0.44	C
	MOTA				116	0.352	40.983	36.451	1.00	0.44	0
20	ATOM ATOM				116	-4.340 -6.838	40.999 41.795	34.057 35.343	1.00	0.00	H H
2.0	ATOM				116	-5.732	40.521	37.186	1.00	0.00	н
	MOTA	4566 21			116	-5.607	42.248	37.523	1.00	0.00	H
	ATOM	4567 1	HD1 TY	R B	116	-3.439	43.399	37.135	1.00	0.00	H
0.5	ATOM				116	-3.838	39.248	36.357	1.00	0.00	H
25	MOTA				116	-0.986 -1.421	43.139	37.108 36.180	1.00	0.00	H
	MOTA MOTA				116	0.572	39.030 40.183	35.940	1.00	0.00	H H
	ATOM				117	-5.625	44.154	35.689	1.00	0.45	N
	ATOM			S B	117	-5.196	45.486	35.366	1.00	0.45	С
30	ATOM				117	-5.361	45.714	33.903	1.00	0.45	Ç
	ATOM				117	-4.381	45.874	33.177	1.00	0.45	0
	ATOM ATOM				117	-3.732 -3.486	45.803 46.035	35.716 37.205	1.00 1.00	0.45 0.45	C
	ATOM				117	-2.021	46.314	37.540	1.00	0.45	č
35	MOTA				117	-1.803	46.773	38.982	1.00	0.45	C
	ATOM	4580	NZ LY	SB	117	-1.648	45.598	39.868	1.00	0.45	N1+
	ATOM				117	-6.473	44.044	36.231	1.00	0.00	H
	ATOM				117	-5.857	46.181	35.904	1.00	0.00	H
40	ATOM ATOM	4583 1F 4584 2F			117	-3.423 -3.072	46.732 45.012	35.202 35.321	1.00	0.00	H H
30	ATOM	4585 11			117	-4.032	45.396	37.906	1.00	0.00	H
	ATOM	4586 2F			117	-3.730	47.063	37.280	1.00	0.00	H
	MOTA	4587 1H			117	-1.662	47.096	36.845	1.00	0.00	H
4 5	ATOM	4588 2F			117	-1.404	45.426	37.399	1.00	0.00	H
45	ATOM	4589 1F 4590 2F			117	-2.615 -0.875	47.410 47.361	39.361 39.082	1.00	0.00	H H
	MOTA MOTA	4591 1H			117	-1.543	45.856	40.843	1.00	0.00	H
	ATOM	4592 21			117	-2.458	44.990	39.832	1.00	0.00	H
	ATOM	4593 3F			117	-0.847	45.024	39.642	1.00	0.00	H
50	ATOM				118	-6.621	45.732	33.433	1.00	0.21	N
	ATOM	4595 C			118	-6.873	45.917	32.037	1.00	0.21	C C
	ATOM ATOM				118 118	-7.212 -7.958	47.354 47.964	31.806 32.569	1.00 1.00	0.21 0.21	o
	MOTA				118	-8.032	45.104	31.546	1.00	0.21	č
55	ATOM		G1 VA			-8.313	45.486	30.088	1.00	0.21	С
	ATOM		G2 VA			-7.708	43.615	31.749	1.00	0.21	С
	MOTA	4601 H			118	-7.436	45.659	34.029	1.00	0.00	H
	ATOM ATOM				118 118	-5.985 -8.930	45.589 45.345	31.488 32.142	1.00	0.00	H H
60	MOTA	4604 1H				-9.124	44.854	29.695	1.00	0.00	H
00	ATOM	4605 2H				-8.627	46.530	29.946	1.00	0.00	H
	MOTA	4606 3H				-7.398	45.279	29.526	1.00	0.00	H
	MOTA	4607 1H				-8.494	42.960	31.340	1.00	0.00	H
65	ATOM	4608 2H				-6.771	43.353	31.231	1.00	0.00	H
65	ATOM	4609 3H 4610 N			118 119	-7.597 -6.636	43.351 47.944	32.813 30.739	1.00 1.00	0.00 0.09	H N
	MOTA MOTA				119	-6.937	49.309	30.739	1.00	0.09	C
	ATOM	4612 C			119	-7.363	49.370	29.005	1.00	0.09	č
	ATOM				119	-6.814	48.678	28.149	1.00	0.09	0
70	ATOM				119	-5.765	50.232	30.583	1.00	0.09	C
	ATOM	4615 C	G1 IL	ЕВ	119	-5.244	50.204	32.028	1.00	0.09	С

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	ATOM ATOM	4616 CG 4617 CI	32 ILE B 11 01 ILE B 11			30.108 32.199	1.00	0.09	C C
	ATOM	4618 H	ILE B 11	9 -5.959	47.463	30.152	1.00	0.00	н
-	ATOM	4619 H				31.079	1.00	0.00	H
5	MOTA	4620 HE				29.921	1.00	0.00	H
	MOTA MOTA		31 ILE B 11 31 ILE B 11			32.385	1.00	0.00	H
	ATOM	4623 1HG				32.619 30.381	1.00	0.00	H H
	MOTA	4624 2HG				29.021	1.00	0.00	H
10	MOTA	4625 3HG				30.599	1.00	0.00	H
	ATOM	4626 1HD				33.256	1.00	0.00	H
	ATOM ATOM	4627 2HD 4628 3HD	1 ILE B 11 1 ILE B 11			31.623	1.00	0.00	H
	ATOM	4629 N	TYR B 12		51.955 50.200	31.943 28.722	1.00	0.00	H N
15	ATOM	4630 CA				27.377	1.00	0.09	č
	MOTA	4631 C	TYR B 12		51.707	26.923	1.00	0.09	Ċ
	ATOM	4632 0	TYR B 12		52.691	27.658	1.00	0.09	0
	MOTA	4633 CB			50.372	27.212	1.00	0.09	C
20	ATOM ATOM	4634 CG 4635 CD	TYR B 12 1 TYR B 12		48.963 48.235	27.189 28.339	1.00	0.09	C
20	ATOM	4636 CD			48.374	25.973	1.00	0.09	C C
	ATOM		1 TYR B 12		46.937	28.266	1.00	0.09	č
	MOTA	4638 CE			47.081	25.893	1.00	0.09	С
25	ATOM	4639 CZ			46.361	27.043	1.00	0.09	С
25	MOTA MOTA	4640 OH 4641 H	TYR B 12		45.034	26.949	1.00	0.09	0
	ATOM	4642 HA			50.823 49.584	29.425 26.738	1.00	0.00	H H
	ATOM	4643 1HB	TYR B 12		50.876	26.261	1.00	0.00	H
20	MOTA	4644 2HB	TYR B 12		50.971	28.003	1.00	0.00	H
30	ATOM		1 TYR B 120		48.686	29.294	1.00	0.00	H
	MOTA MOTA	4646 HD 4647 HE			48.938 46.356	25.055 29.175	1.00	0.00	H
	ATOM	4648 HE			46.651	24.941	1.00	0.00	H H
	MOTA	4649 HH	TYR B 12		44.595	27.775	1.00	0.00	н
35	MOTA	4650 N	TYR B 12:		51.760	25.689	1.00	0.18	N
	ATOM	4651 CA	TYR B 121		52.999	25.199	1.00	0.18	С
	ATOM ATOM	4652 C 4653 O	TYR B 123		53.324 52.449	23.925 23.108	1.00	0.18 0.18	C 0
	ATOM	4654 CB	TYR B 12		52.937	24.877	1.00	0.18	Ċ
40	MOTA	4655 CG	TYR B 123		52.647	26.150	1.00	0.18	č
	MOTA	4656 CD			53.668	26.987	1.00	0.18	С
	ATOM	4657 CD			51.349	26.509	1.00	0.18	C
	ATOM ATOM	4658 CE:			53.397 51.074	28.160 27.679	1.00	0.18 0.18	C C
45	ATOM	4660 CZ	TYR B 121		52.098	28.506	1.00	0.18	č
	MOTA	4661 OH	TYR B 121	-3.059	51.815	29.707	1.00	0.18	0
	MOTA	4662 H	TYR B 121		50.943	25.120	1.00	0.00	H
	MOTA ATOM	4663 HA	TYR B 121		53.759	25.960	1.00	0.00	H
50	ATOM	4664 1HB 4665 2HB	TYR B 121		53.911 52.184	24.460 24.103	1.00 1.00	0.00	H H
	MOTA		TYR B 121		54.701	26.707	1.00	0.00	Н
	ATOM		TYR B 121		50.534	25.848	1.00	0.00	H
	MOTA		TYR B 121		54.220	28.783	1.00	0.00	H
55	ATOM ATOM		TYR B 121 TYR B 121		50.026	27.774	1.00	0.00	H
33	ATOM	4670 HH 4671 N	LYS B 122		52.351 54.617	29.616 23.757	1.00 1.00	0.00 0.28	H N
	ATOM	4672 CA	LYS B 122		55.139	22.598	1.00	0.28	c
	MOTA	4673 C	LYS B 122		56.236	22.126	1.00	0.28	С
60	ATOM	4674 0	LYS B 122		57.264	22.790	1.00	0.28	0
60	MOTA MOTA	4675 CB	LYS B 122		55.804	22.933	1.00	0.28	C
	ATOM	4676 CG 4677 CD	LYS B 122 LYS B 122		56.243 56.836	21.722 22.111	1.00	0.28	C
	ATOM	4678 CE	LYS B 122	-13.183	56.151	23.316	1.00	0.28	c
	ATOM	4679 NZ	LYS B 122	-14.483	56.791	23.628	1.00	0.28	N1+
65	MOTA	4680 H	LYS B 122	-8.144	55.299	24.484	1.00	0.00	H
	ATOM	4681 HA	LYS B 122	-9.164	54.338	21.865	1.00	0.00	H
	MOTA MOTA	4682 1HB 4683 2HB	LYS B 122 LYS B 122	-10.242 -10.988	56.625 55.031	23.659 23.342	1.00	0.00	H H
	ATOM	4684 1HG	LYS B 122	-10.300	55.374	23.342	1.00	0.00	H H
70	MOTA	4685 2HG	LYS B 122	-10.623	56.984	21.114	1.00	0.00	H
	MOTA	4686 1HD	LYS B 122	-13.201	56.854	21.232	1.00	0.00	H

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ATOM 4687 2HD LYS B 122 -12.369 57.894 22.385 1.00 0.00 ATOM H 4688 1HE LYS B 122 -12.551 56.319 24.190 1.00 0.00 H ATOM 4689 2HE LYS B 122 -13.425 55.120 23.185 0.00 1.00 ATOM 4690 1HZ LYS B 122 -14.924 56.393 24.445 5 1.00 0.00 н MOTA 4691 2HZ LYS B 122 -14.393 57.785 23.789 1.00 0.00 H MOTA 4692 3HZ LYS B 122 -15.134 56.665 22.860 1.00 0.00 Н MOTA 4693 N ASP B 123 -7.464 56.040 20.965 1.00 0.20 N MOTA 4694 ASP B 123 CA -6.591 57.040 20.428 1.00 0.20 C MOTA 4695 С ASP B 123 -5.595 57.437 21.470 1.00 0.20 10 C ATOM 4696 0 ASP B 123 -5.193 58.597 21.556 1.00 0.20 0 ATOM 4697 CB ASP B 123 -7.339 58.273 19.901 1.00 0.20 ASP B 123 ATOM 4698 CG -8.044 57.821 18.631 1.00 0.20 C OD1 ASP B 123 ATOM 4699 -7.553 56.845 18.001 1.00 0.20 0 MOTA 4700 OD2 ASP B 123 -9.081 58.436 18.274 1.00 15 0.20 01 ATOM 4701 H **ASP B 123** -7.659 55.230 20.379 1.00 0.00 H HA ATOM 4702 ASP B 123 -5.967 56.577 19.640 1.00 0.00 H MOTA 4703 1HB ASP B 123 -6.613 59.051 19.613 1.00 0.00 H ATOM 4704 2HB **ASP B 123** -8.032 58.726 20.624 1.00 0.00 H MOTA 4705 N **GLY B 124** -5.173 56.462 22.296 1.00 0.17 20 N ATOM 4706 CA **GLY B 124** -4.147 56.707 23.266 1.00 0.17 C GLY B 124 MOTA 4707 C -4.739 57.254 24.523 1.00 0.17 C MOTA 4708 ٥ **GLY B 124** -4.011 57.600 25.454 1.00 0.17 0 ATOM 4709 Н **GLY B 124** -5.500 55.518 22.162 1.00 0.00 Н MOTA 4710 1HA **GLY B 124** -3.397 57.414 22.878 1.00 25 0.00 H GLY B 124 MOTA 4711 2HA -3.641 55.758 23.511 1.00 0.00 H 4712 MOTA **GLU B 125** N -6.076 57.350 24.601 1.00 0.24 N ATOM 4713 CA **GLU B 125** -6.638 57.879 25.806 1.00 0.24 C ATOM 4714 **GLU B 125** С -7.229 56.729 26.552 1.00 0.24 С MOTA 4715 GLU B 125 0 -7.934 55.904 25.980 30 1.00 0.24 0 MOTA 4716 CB **GLU B 125** -7.747 58.908 25.550 1.00 0.24 C MOTA 4717 CG **GLU B 125** -8.099 59.729 26.785 1.00 0.24 С ATOM 4718 CD **GLU B 125** -9.183 60.720 26.392 1.00 0.24 C MOTA 4719 OE1 GLU B 125 -10.013 60.366 25.512 1.00 0.24 0 MOTA 4720 OE2 GLU B 125 -9.192 61.843 26.962 1.00 0.24 35 ATOM 01 4721 H **GLU B 125** -6.663 57.298 23.773 1.00 0.00 Н ATOM 4722 HA **GLU B 125** -5.870 58.399 26.400 1.00 0.00 H GLU B 125 ATOM 4723 1HB -8.638 58.390 25.156 1.00 0.00 Н MOTA 4724 2HB GLU B 125 -7.408 59.599 24.755 1.00 0.00 H ATOM 4725 1HG **GLU B 125** -7.225 60.253 27.203 1.00 40 0.00 H ATOM 4726 2HG GLU B 125 -8.494 59.077 27.582 1.00 0.00 ALA B 126 ALA B 126 ATOM 4727 N -6.967 56.629 27.865 1.00 0.26 N ATOM 4728 CA -7.483 55.489 28.563 1.00 0.26 С MOTA 4729 C ALA B 126 -8.923 55.737 28.870 1.00 0.26 C ATOM 4730 0 ALA B 126 -9.257 56.616 29.662 1.00 45 0.26 0 ATOM 4731 ALA B 126 CB -6.771 55.212 29.898 1.00 0.26 C ATOM 4732 ALA B 126 H -6.347 57.258 28.348 1.00 0.00 Н ATOM 4733 HA **ALA B 126** -7.283 54.612 27.943 1.00 0.00 Н ATOM 4734 1HB -7.245 **ALA B 126** 54.340 30.375 1.00 0.00 Н ATOM -5.708 54.984 4735 2HB ALA B 126 29.733 1.00 50 0.00 H ATOM 4736 3HB ALA B 126 -6.835 56.063 30.593 1.00 0.00 H ATOM 4737 N **LEU B 127** -9.819 54.977 28.210 1.00 0.39 N ATOM 4738 CA **LEU B 127** -11.223 55.120 28.455 1.00 0.39 С MOTA 4739 **LEU B 127** С -11.504 54.659 29.846 1.00 0.39 C ATOM 4740 0 **LEU B 127** -12.150 55.361 30.622 1.00 0.39 55 0 ATOM 4741 -12.082 54.243 CB **LEU B 127** 27.532 1.00 0.39 С MOTA 4742 CG **LEU B 127** -11.973 54.616 26.046 1.00 0.39 С MOTA 4743 CD1 LEU B 127 -10.541 54.413 25.527 1.00 0.39 С MOTA 4744 CD2 LEU B 127 -13.021 53.865 25.210 1.00 0.39 C ATOM -9.482 4745 H **LEU B 127** 54.256 27.585 1.00 60 0.00 LEU B 127 MOTA 4746 HA -11.515 56.177 28.359 1.00 0.00 Н MOTA 4747 1HB **LEU B 127** -13.130 54.364 27.866 1.00 0.00 MOTA Н 4748 2HB **LEU B 127** -11.833 53.177 27.665 1.00 0.00 ATOM 4749 HG **LEU B 127** -12.194 55.696 26.007 1.00 0.00 н 4750 1HD1 LEU B 127 MOTA -10.536 53.792 24.623 65 1.00 0.00 H MOTA 4751 2HD1 LEU B 127 55.385 -10.073 25.396 1.00 0.00 Н ATOM 4752 3HD1 LEU B 127 -9.942 53.772 26.170 1.00 0.00 H 4753 1HD2 LEU B 127 MOTA -12.582 54.000 24.252 1.00 0.00 H ATOM 4754 2HD2 LEU B 127 -13.035 52.790 25.442 1.00 0.00 Н ATOM 4755 3HD2 LEU B 127 -14.037 54.274 25.281 1.00 70 0.00 Н ATOM 4756 N LYS B 128 -11.008 53.457 30.209 1.00 0.43 ATOM 4757 CA LYS B 128 -11.294 52.985 31.530 1.00 0.43

5	MOTA MOTA MOTA MOTA MOTA MOTA MOTA	4759 4760 4761 4762 4763 4764	O LYS CB LYS CG LYS CD LYS CE LYS NZ LYS	B 128	-9.524 -12.614 -12.560 -13.718 -13.540	51.449 52.207 50.838 49.918 48.478	31.122 31.641 30.960 31.350 30.872	1.00 1.00 1.00 1.00	0.43 0.43 0.43 0.43	C O C C C N1+
10	MOTA MOTA MOTA MOTA MOTA		HB LYS	B 128 B 128 B 128		53.843 52.810 52.073	32.227 31.235 32.717	1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
15	ATOM ATOM ATOM ATOM ATOM	4770 21 4771 11 4772 21 4773 11 4774 21	iG LYS iD LYS iD LYS iE LYS	B 128	-12.473 -14.667 -13.841 -13.239 -14.468	50.978 50.313 49.922	29.880 30.950 32.449 29.841 31.072	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н
20	ATOM ATOM ATOM ATOM ATOM	4775 11 4776 21 4777 31 4778 1	IZ LYS IZ LYS IZ LYS I TYR	B 128	-12.368 -11.541 -12.592 -10.043 -9.095	46.844	31.429 31.441 32.634 33.275	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H N
25	ATOM ATOM ATOM ATOM ATOM	4780 C 4781 C 4782 C 4783 C	TYR TYR TYR	B 129 B 129 B 129 B 129	-9.784 -10.405 -7.861 -7.171 -6.375	50.262 50.879 51.683 50.706 49.701	33.832 34.940 35.803 34.435 35.325	1.00 1.00 1.00 1.00	0.26 0.26 0.26 0.26	00000
30	MOTA ATOM ATOM MOTA MOTA	4785 C 4786 C 4787 C 4788 C	D2 TYR E1 TYR E2 TYR Z TYR	B 129 B 129	-7.327 -5.750 -6.707 -5.916 -5.283	50.815 48.816 49.936 48.935 48.036	34.823 36.687 35.674 37.540 37.035	1.00 1.00 1.00 1.00	0.26 0.26 0.26 0.26	00000
35	ATOM ATOM ATOM ATOM ATOM	4790 H 4791 H 4792 1H 4793 2H	TYR A TYR B TYR	B 129 B 129 B 129 B 129	-10.607 -8.771 -8.174 -7.213	52.393 50.291 52.568 52.072	37.916 33.952 33.049 35.013 33.637	1.00 1.00 1.00 1.00	0.26 0.00 0.00 0.00	0 H H H
40	MOTA MOTA MOTA MOTA	4795 H 4796 H 4797 H 4798 H	D2 TYR E1 TYR E2 TYR H TYR	B 129 B 129 B 129 B 129	-6.453 -7.952 -5.114 -6.841 -5.832	49.410 51.605 48.061 50.075 47.984	33.799 37.097 35.238 38.607 38.711	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
45	ATOM ATOM ATOM ATOM ATOM	4799 N 4800 C 4801 C 4802 O 4803 C	A TRP TRP TRP TRP	B 130 B 130 B 130 B 130 B 130	-9.712 -10.311 -9.437 -8.929 -11.716	48.916 48.181 46.987 46.405 47.655	34.931 36.006 36.219 35.261 35.683	1.00 1.00 1.00 1.00	0.16 0.16 0.16 0.16 0.16	и С О С
50	MOTA MOTA MOTA MOTA	4806 CI 4807 NI 4808 CI	01 TRP	B 130 B 130	-12.467 -12.409 -13.463 -13.299 -13.957	47.127 45.906 47.882 45.859 47.066	36.882 37.486 37.588 38.532 38.603	1.00 1.00 1.00 1.00	0.16 0.16 0.16 0.16 0.16	С С С
55	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4810 C	TRP	B 130	-13.932 -14.932 -14.913 -15.404 -9.108 -10.329	49.151 47.506 49.593 48.787 48.407 48.805	37.402 39.452 38.264 39.270 34.292 36.916	1.00 1.00 1.00 1.00 1.00	0.16 0.16 0.16 0.16 0.00	С С Н Н
60	ATOM ATOM ATOM ATOM ATOM	4815 1HE 4816 2HE 4817 HE 4818 HE	TRP	B 130 B 130 B 130 B 130	-11.622 -12.306 -11.644 -13.577 -13.550	46.878 48.463 45.253 45.048 49.803	34.909 35.220 37.343 39.057 36.623	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
65	ATOM ATOM ATOM ATOM ATOM	4820 Hz 4821 Hz	2 TRP 1 3 TRP 1 2 TRP 1 TYR 1	B 130 B 130	-15.318 -15.309 -16.179 -9.204	46.865 50.600 49.170 46.599	40.242 38.152 39.930 37.487	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00 0.17	H H H N
70	ATOM ATOM ATOM ATOM	4825 C 4826 O 4827 CB 4828 CG	TYR I	3 131 3 131 3 131	-8.351 -8.991 -8.436 -8.087 -7.166	45.465 44.235 43.582 45.152 46.173	37.683 37.120 36.238 39.164 39.731	1.00 1.00 1.00	0.17 0.17 0.17 0.17 0.17	0000

	ATOM ATOM ATOM ATOM	4830 (4831 (D1 TYR B 1: D2 TYR B 1: E1 TYR B 1:	31 -5.84 31 -6.75	4 45.857 4 48.358	39.937 40.602	1.00	0.17 0.17	c c
5	ATOM ATOM ATOM ATOM	4833 C 4834 C 4835 H	E2 TYR B 13 EZ TYR B 13 EH TYR B 13 E TYR B 13 EA TYR B 13	31 -5.433 31 -4.543 31 -9.633	3 48.034 2 48.984 3 47.043	40.800 41.345 38.280	1.00 1.00 1.00	0.17 0.17 0.17 0.00 0.00	и О С
10	ATOM ATOM ATOM ATOM	4840 H	B TYR B 13 B TYR B 13 D1 TYR B 13 D2 TYR B 13	31 -7.635 31 -9.022 31 -8.663 31 -5.494	5 44.147 2 45.099 7 47.686	39.216 39.746 39.973	1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H H
15	MOTA MOTA MOTA MOTA MOTA	4842 H 4843 H 4844 N	GLU B 13	11 -3.963 11 -5.050 12 -10.189	46.496 49.530 43.889	40.710 41.957 37.630	1.00 1.00 1.00	0.00 0.00 0.00 0.19	H H H N
20	ATOM ATOM ATOM ATOM	4846 C 4847 O 4848 C 4849 C	GLU B 13 GLU B 13 B GLU B 13	2 -11.520 2 -11.501 2 -11.851	42.727 41.741 42.161	35.909 35.175	1.00 1.00 1.00 1.00	0.19 0.19 0.19 0.19 0.19	00000
25	ATOM ATOM ATOM ATOM	4852 O	D GLU B 13 E1 GLU B 13 E2 GLU B 13 GLU B 13	2 -13.838 2 -14.098 2 -14.202 2 -10.574	42.479 41.248 43.236 44.356	39.702 39.651 40.641 38.433	1.00 1.00 1.00 1.00	0.19 0.19 0.19 0.00	с о о1- н
30	ATOM ATOM ATOM ATOM ATOM	4854 H 4855 1H 4856 2H 4857 1H 4858 2H	GLU B 13 GLU B 13 GLU B 13	2 -11.321 2 -12.189 2 -13.639	41.965 41.177 43.344	37.149 39.245 37.919 37.692	1.00 1.00 1.00	0.00 0.00 0.00	н н н
	ATOM ATOM ATOM ATOM	4859 N 4860 CJ 4861 C 4862 O	ASN B 13	3 -12.116 3 -12.974 3 -12.209	43.878 43.903 43.857	39.059 35.539 34.382 33.098 32.738	1.00 1.00 1.00 1.00	0.00 0.18 0.18 0.18	H N C C
35	ATOM ATOM ATOM	4866 NI	F ASN B 13: 01 ASN B 13: 02 ASN B 13:	3 -13.907 3 -14.988 3 -14.893 3 -16.041	45.129 44.843	34.320 33.284 32.522 33.248	1.00 1.00 1.00 1.00	0.18 0.18 0.18 0.18	C C O N
40	MOTA MOTA MOTA MOTA	4867 H 4868 HA 4869 1HE 4870 2HE	ASN B 133	3 -13.641 3 -13.387 3 -14.388	44.684 43.023 46.056 45.278	36.122 34.482 34.048 35.302	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
45	ATOM ATOM ATOM ATOM ATOM	4871 IHL 4872 2HD 4873 N 4874 CA 4875 C	2 ASN B 133 12 ASN B 133 HIS B 134 HIS B 134 HIS B 134	3 -16.734 -12.358 -11.782	46.456 45.541 42.718 42.426	33.904 32.536 32.393 31.111	1.00 1.00 1.00	0.00 0.00 0.16 0.16	H H N C
50	ATOM ATOM ATOM ATOM	4876 O 4877 CB 4878 CG 4879 ND	HIS B 134 HIS B 134 HIS B 134 1 HIS B 134	-11.908 -11.845 -11.133 -9.767	43.153 43.530 40.927 40.093 39.912	30.020 29.016 30.781 31.803 31.837	1.00 1.00 1.00 1.00	0.16 0.16 0.16 0.16 0.16	C C C N
55	ATOM ATOM ATOM ATOM ATOM ATOM	4881 CE	2 HIS B 134 1 HIS B 134 2 HIS B 134 HIS B 134 HIS B 134 HIS B 134	-9.506 -10.603 -12.816 -10.736	39.390 39.115 38.772 41.946 42.768 40.786	32.858 32.903 33.554 32.852 31.094 29.778	1.00 1.00 1.00 1.00 1.00	0.16 0.16 0.16 0.00 0.00	C C N H H
60	ATOM ATOM ATOM ATOM ATOM	4888 HE	HIS B 134 2 HIS B 134 1 HIS B 134 2 HIS B 134	-12.890 -12.657 -8.543 -10.667	40.590 39.288 38.682 38.227	30.715 33.175 33.088 34.389	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
65	MOTA MOTA MOTA MOTA	4891 CA 4892 C 4893 O 4894 CB	ASN B 135 ASN B 135 ASN B 135	-14.631 -14.941 -14.867 -15.986	43.359 43.884 45.332 45.856 43.176	30.179 29.100 29.306 30.416 28.963	1.00 1.00 1.00	0.14 0.14 0.14 0.14 0.14	N C C O C
70	ATOM ATOM ATOM ATOM ATOM		ASN B 135 ASN B 135 ASN B 135 ASN B 135 ASN B 135	-15.720 -15.032 -16.270 -14.277 -14.091	40.813 43.286	28.665 27.704 29.528 31.091 28.156	1.00 1.00 1.00 1.00	0.14 0.14 0.14 0.00	C N H H

	ATOM	4900 1HE				28.112	1.00	0.00	н
	ATOM ATOM	4901 2HE	ASN B 135 2 ASN B 135	-16.609				0.00	H
	ATOM		2 ASN B 135					0.00	H H
5	ATOM	4904 N	ILE B 136					0.19	N
	ATOM	4905 CA						0.19	Ĉ
	ATOM	4906 C	ILE B 136					0.19	С
	MOTA MOTA	4907 O 4908 CB	ILE B 136				1.00	0.19	0
10	ATOM		1 ILE B 136			27.694 27.966	1.00	0.19 0.19	C
	MOTA		2 ILE B 136			26.207		0.19	c
	ATOM		1 ILE B 136			27.751	1.00	0.19	c
	ATOM	4912 H	ILE B 136			27.283	1.00	0.00	H
15	ATOM ATOM	4913 HA 4914 HB	ILE B 136			29.234	1.00	0.00	H
10	ATOM		1 ILE B 136			28.141 28.996	1.00 1.00	0.00	H
	ATOM		1 ILE B 136		50.096	27.307	1.00	0.00	H H
	ATOM	4917 1HG	2 ILE B 136	-13.544	48.610	25.812	1.00	0.00	H
20	MOTA		2 ILE B 136		46.948	26.193	1.00	0.00	H
20	ATOM		2 ILE B 136	_	48.283	25.560	1.00	0.00	H
	MOTA ATOM		1 ILE B 136 1 ILE B 136		51.752	28.250	1.00	0.00	H
	ATOM		1 ILE B 136	-13.745	50.375 50.990	28.101 26.675	1.00	0.00	H H
	MOTA	4923 N	SER B 137	-17.788	48.414	27.604	1.00	0.24	N
25	MOTA	4924 CA	SER B 137	-18.920	48.568	26.741	1.00	0.24	Ĉ
	ATOM	4925 C	SER B 137	-19.203	50.029	26.610	1.00	0.24	С
	ATOM ATOM	4926 O 4927 CB	SER B 137 SER B 137	-19.102	50.781	27.577	1.00	0.24	0
	ATOM	4928 OG	SER B 137	-20.185 -21.276	47.894 48.071	27.299 26.411	1.00	0.24	C
30	ATOM	4929 H	SER B 137	-17.726	49.066	28.368	1.00	0.24	O H
	ATOM	4930 HA	SER B 137	-18.674	48.121	25.782	1.00	0.00	H
	MOTA	4931 1HB	SER B 137	-20.436	48.283	28.302	1.00	0.00	н
	MOTA	4932 2HB	SER B 137	-20.027	46.813	27.395	1.00	0.00	H
35	ATOM ATOM	4933 HG 4934 N	SER B 137 ILE B 138	-21.483 -19.553	49.017	26.401	1.00	0.00	H
55	ATOM	4935 CA	ILE B 138	-19.333	50.475 51.857	25.389 25.203	1.00 1.00	0.31 0.31	N C
	ATOM	4936 C	ILE B 138	-21.299	51.893	24.779	1.00	0.31	c
	MOTA	4937 O	ILE B 138	-21.688	51.253	23.804	1.00	0.31	ŏ
40	MOTA	4938 CB	ILE B 138	-19.075	52.508	24.114	1.00	0.31	С
40	MOTA MOTA		ILE B 138	-17.571 -19.578	52.405	24.424	1.00	0.31	C
	ATOM		ILE B 138	-16.674	53.954 52.719	23.962 23.229	1.00 1.00	0.31 0.31	C
	ATOM	4942 H	ILE B 138	-19.600	49.853	24.587	1.00	0.00	н
4 -	ATOM	4943 HA	ILE B 138	-19.710	52.421	26.135	1.00	0.00	н
45	ATOM	4944 HB	ILE B 138	-19.268	52.008	23.155	1.00	0.00	H
	ATOM ATOM		ILE B 138	-17.316 -17.308	51.376 53.049	24.735	1.00	0.00	H
	ATOM		ILE B 138	-18.854	54.629	25.281 23.492	1.00 1.00	0.00	H H
_	ATOM		ILE B 138	-20.505	54.001	23.368	1.00	0.00	H
50	MOTA		ILE B 138	-19.788	54.411	24.944	1.00	0.00	H
	ATOM		ILE B 138	-15.696	52.223	23.340	1.00	0.00	H
ŕ	ATOM ATOM		ILE B 138 ILE B 138		52.364 53.793			0.00	H
	ATOM	4953 N	THR B 139	-16.455 -22.134	52.652	23.163 25.502	1.00	0.00	H
55	ATOM	4954 CA	THR B 139	-23.515	52.679	25.136	1.00	0.40	N C
	ATOM	4955 C	THR B 139	-23.749	53.927	24.359	1.00	0.40	č
	ATOM	4956 O	THR B 139	-23.036	54.914	24.535	1.00	0.40	0
	MOTA	4957 CB	THR B 139	-24.443	52.677	26.311	1.00	0.40	С
60	ATOM ATOM		THR B 139 THR B 139	-24.163 -24.261	53.789 51.362	27.147	1.00	0.40	0
00	ATOM	4960 H	THR B 139	-21.877	53.234	27.085 26.282	1.00	0.40	C H
	ATOM	4961 HA	THR B 139	-23.767	51.798	24.523	1.00	0.00	H
	ATOM	4962 HB	THR B 139	-25.487	52.734	25.945		0.00	H
65	ATOM		THR B 139	-24.403	54.588	26.652	1.00	0.00	H
65	ATOM		THR B 139	-24.978	51.292	27.920		0.00	H
	ATOM ATOM	4965 2HG2	THR B 139 THR B 139	-24.420 -23.251	50.485 51.293	26.436 27.520		0.00	H
	ATOM	4967 N	ASN B 140	-23.251	53.894	23.470		0.00 0.29	H N
	ATOM	4968 CA	ASN B 140	-25.086	55.022	22.647		0.29	Č
70	MOTA	4969 C	ASN B 140	-23.840	55.522	21.994		0.29	č
	ATOM	4970 O	ASN B 140	-23.385	56.631	22.272	1.00	0.29	0

5 ATOM 4976 HA ASN B 140 -25.331 S3 082 23.683 1.00 0.00 HA ATOM 4977 HB ASN B 140 -25.766 57.075 22.770 1.00 0.00 HA ATOM 4977 HB ASN B 140 -25.766 57.075 22.770 1.00 0.00 HA ATOM 4978 ZHB ASN B 140 -25.736 57.075 22.770 1.00 0.00 HA ATOM 4991 ZHD ASN B 140 -27.995 57.144 22.347 1.00 0.00 HA ATOM 4990 ZHD ASN B 140 -27.995 57.144 22.347 1.00 0.00 HA ATOM 4991 DATOM 4991 DATOM 4991 DATOM 4991 DATOM 4991 DATOM 4992 CA ALA B 141 -22.202 55.066 20.453 1.00 0.26 CA ATOM 4992 CA ALA B 141 -22.202 55.066 20.453 1.00 0.26 CA ATOM 4998 DATOM 4992 CA ALA B 141 -22.259 56.305 19.562 1.00 0.26 CA ATOM 4996 CA ALA B 141 -22.259 56.305 19.562 1.00 0.26 CA ATOM 4998 DATOM 4996 CA ALA B 141 -22.259 56.305 19.206 1.00 0.26 CA ATOM 4998 DATOM 4996 CA ALA B 141 -23.357 53.762 20.926 1.00 0.26 CA ATOM 4998 DATOM 4996 DATO	_	ATOM ATOM ATOM ATOM			N B	140	-27.131	55.764 54.884	23.832 24.671	1.00	0.29	C C O N
ATOM 4980 ZMID2 ASN B 140 -29,087 56,156 23,487 1,00 0.00 1	5	ATOM ATOM ATOM	4976 4977 4978	HA AS 1HB AS 2HB AS	N B N B N B	140 140 140	-25.351 -25.796 -25.766 -25.173	53.083 54.687 57.075 56.460	23.363 21.874 22.770 24.334	1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н
ATOM	10	ATOM ATOM ATOM	4980 : 4981 4982	PHD2 AS: N AL CA AL	N B A B A B	140 141 141	-29.087 -23.250 -22.029	56.156 54.699 55.068	23.487 21.107 20.453	1.00 1.00 1.00	0.00 0.26 0.26	N C
ATOM 4989 2HB ALA B 141 -21.267 53.060 20.048 1.00 0.00 H	15	MOTA MOTA MOTA	4985 4986 4987	CB ALI H ALI HA ALI	AB AB AB	141 141 141	-21.490 -23.587 -21.258	53.988 53.762 55.258	19.206 19.499 20.926 21.225	1.00 1.00 1.00	0.26 0.26 0.00 0.00	0 C H H
25 ATOM 4995 CB THR B 142 -19.288 57.465 17.779 1.00 0.35 CO ATOM 4995 CB THR B 142 -21.175 59.547 19.617 1.00 0.35 CO ATOM 4996 CG1 THR B 142 -21.175 59.547 19.617 1.00 0.35 CO ATOM 4998 H THR B 142 -21.964 50.721 18.859 1.00 0.35 CO ATOM 4998 H THR B 142 -22.265 56.794 19.709 1.00 0.00 H ATOM 4998 H THR B 142 -22.265 56.794 19.709 1.00 0.00 H ATOM 5000 HB THR B 142 -22.222 58.374 18.164 1.00 0.00 H ATOM 5001 HG1 THR B 142 -21.924 59.484 20.430 1.00 0.00 H ATOM 5001 HG1 THR B 142 -21.924 59.484 20.430 1.00 0.00 H ATOM 5001 HG1 THR B 142 -19.677 60.411 20.966 1.00 0.00 H ATOM 5001 3HC2 THR B 142 -19.545 58.677 20.799 1.00 0.00 H ATOM 5003 2HC2 THR B 142 -19.025 59.711 19.495 1.00 0.00 H ATOM 5005 N VAL B 143 -20.067 59.427 16.968 1.00 0.29 C ATOM 5006 CA VAL B 143 -19.038 59.595 15.985 1.00 0.29 C ATOM 5009 CB VAL B 143 -19.038 59.595 15.985 1.00 0.29 C ATOM 5001 CG1 VAL B 143 -19.038 59.595 16.6800 1.00 0.29 C ATOM 5011 CG2 VAL B 143 -19.266 60.803 15.127 1.00 0.29 C ATOM 5011 CG2 VAL B 143 -19.266 60.803 15.127 1.00 0.29 C ATOM 5011 CG2 VAL B 143 -19.266 60.803 15.127 1.00 0.29 C ATOM 5011 CG2 VAL B 143 -19.266 60.803 15.127 1.00 0.29 C ATOM 5013 HA VAL B 143 -19.266 60.803 15.127 1.00 0.29 C ATOM 5014 HB VAL B 143 -19.266 60.803 15.329 1.00 0.00 H ATOM 5016 2HC1 VAL B 143 -19.266 60.803 15.327 1.00 0.29 C ATOM 5017 HW VAL B 143 -19.266 60.803 15.327 1.00 0.00 H ATOM 5016 2HC1 VAL B 143 -19.266 60.803 13.377 1.00 0.00 H ATOM 5016 2HC1 VAL B 143 -19.266 60.803 13.377 1.00 0.00 H ATOM 5016 2HC1 VAL B 143 -19.266 60.803 13.377 1.00 0.00 H ATOM 5016 2HC1 VAL B 143 -17.126 61.563 13.377 1.00 0.00 H ATOM 5018 1HC2 VAL B 143 -17.126 60.91 13.559 1.00 0.00 H ATOM 5018 1HC2 VAL B 143 -17.126 60.91 13.559 1.00 0.00 H ATOM 5020 CG GG GLU B 144 -14.738 59.159 19.072 1.00 0.25 C ATOM 5030 H GLU B 144 -14.738 59.159 19.072 1.00 0.25 C ATOM 5030 H GLU B 144 -17.266 62.836 19.072 1.00 0.25 C ATOM 5030 H GLU B 144 -17.7460 60.941 19.859 1.00 0.00 H ATOM 5031 HB GLU B 144 -17.7460 60.941 19.859 1.00 0.00 H ATOM 5031 HB GLU B 1	20	MOTA MOTA MOTA MOTA	4989 2 4990 3 4991 4992	HB ALZ HB ALZ N THI CA THI	A B A B R B R B	141 141 142 142	-21.267 -22.201 -21.198 -21.277	53.060 53.762 57.103	20.048 18.690 19.475	1.00 1.00 1.00	0.00 0.00 0.35	H H N
30	25	ATOM ATOM ATOM	4994 4995 4996	O THE CB THE OG1 THE	R B R B	142 142 142	-19.288 -21.175 -21.424	57.465 59.547 60.721	17.779 19.617 18.859	1.00 1.00 1.00	0.35 0.35 0.35	0 C 0
ATOM 5003 2HG2 THR B 142 -19.545 58.677 20.799 1.00 0.00 H ATOM 5004 3HG2 THR B 142 -19.002 59.711 19.495 1.00 0.00 H ATOM 5005 N VAL B 143 -20.067 59.427 16.968 1.00 0.29 C ATOM 5007 C VAL B 143 -19.038 59.595 15.985 1.00 0.29 C ATOM 5007 C VAL B 143 -17.723 59.745 16.680 1.00 0.29 C ATOM 5007 C VAL B 143 -17.723 59.745 16.680 1.00 0.29 C ATOM 5000 CB VAL B 143 -19.256 60.803 15.127 1.00 0.29 C ATOM 5010 CG1 VAL B 143 -19.256 60.803 15.127 1.00 0.29 C ATOM 5010 CG1 VAL B 143 -19.256 60.803 15.127 1.00 0.29 C ATOM 5011 CG2 VAL B 143 -19.256 60.803 15.127 1.00 0.29 C ATOM 5012 H VAL B 143 -20.644 60.686 14.470 1.00 0.29 C ATOM 5012 H VAL B 143 -20.644 60.686 14.470 1.00 0.29 C ATOM 5012 H VAL B 143 -18.850 58.830 15.29 1.00 0.00 H ATOM 5013 HA VAL B 143 -18.850 58.830 15.329 1.00 0.00 H ATOM 5015 HBG VAL B 143 -18.850 58.830 15.329 1.00 0.00 H ATOM 5015 HBG VAL B 143 -18.282 61.693 13.377 1.00 0.00 H ATOM 5015 HBG VAL B 143 -17.142 61.156 14.609 1.00 0.00 H ATOM 5018 HBG VAL B 143 -17.142 61.156 14.609 1.00 0.00 H ATOM 5018 HBG VAL B 143 -20.762 61.156 14.609 1.00 0.00 H ATOM 5018 HBG VAL B 143 -20.762 61.326 13.559 1.00 0.00 H ATOM 5020 3HG2 VAL B 143 -20.762 61.326 13.559 1.00 0.00 H ATOM 5020 3HG2 VAL B 143 -20.762 61.326 13.578 1.00 0.00 H ATOM 5020 3HG2 VAL B 143 -20.762 60.414 17.845 1.00 0.25 C ATOM 5025 CB GLU B 144 -17.728 60.414 17.845 1.00 0.25 C ATOM 5025 CB GLU B 144 -17.728 60.414 17.845 1.00 0.25 C ATOM 5025 CB GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5025 CB GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5023 LHB GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5033 LHB GLU B 144 -17.781 63.464 20.537 1.00 0.00 H ATOM 5031 HA GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5032 LHB GLU B 144 -17.781 63.464 20.537 1.00 0.00 H ATOM 5033 LHB GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5033 CA ASP B 145 -16.438 57.030 19.619 1.00 0.02 C C ATOM 5037 CA ASP B 145 -16.438 57.030 19.619 1.00 0.22 C C ATOM 5039 O ASP B 145 -16.438 57.030 19.619 1.00 0.22 C C ATOM 5030 O ASP B 145 -16.438 5	30	MOTA MOTA MOTA	4999 5000 5001	H THE HA THE HB THE HG1 THE	R B R B R B	142 142 142 142	-20.268 -22.202 -21.924 -20.924	56.794 58.374 59.484 61.441	19.709 18.164 20.430 19.314	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	Н Н Н Н
ATOM 5008 O VAL B 143 -16.696 59.265 16.203 1.00 0.29 C ATOM 5009 CB VAL B 143 -19.256 60.803 15.127 1.00 0.29 C ATOM 5010 CGI VAL B 143 -18.096 60.900 14.122 1.00 0.29 C ATOM 5011 CG2 VAL B 143 -20.644 60.686 144.470 1.00 0.29 C ATOM 5012 H VAL B 143 -20.644 60.686 144.470 1.00 0.29 C ATOM 5013 HA VAL B 143 -20.644 60.686 144.470 1.00 0.00 H ATOM 5013 HA VAL B 143 -18.850 58.830 15.329 1.00 0.00 H ATOM 5015 1HG1 VAL B 143 -18.292 61.693 13.377 1.00 0.00 H ATOM 5015 1HG1 VAL B 143 -19.249 61.727 15.730 1.00 0.00 H ATOM 5016 2HG1 VAL B 143 -17.963 59.961 13.559 1.00 0.00 H ATOM 5016 3HG2 VAL B 143 -17.963 59.961 13.559 1.00 0.00 H ATOM 5018 1HG2 VAL B 143 -17.963 59.961 13.559 1.00 0.00 H ATOM 5010 3HG2 VAL B 143 -20.742 61.326 13.578 1.00 0.00 H ATOM 5020 3HG2 VAL B 143 -20.859 59.656 14.167 1.00 0.00 H ATOM 5020 3HG2 VAL B 143 -21.447 60.987 15.163 1.00 0.00 H ATOM 5020 3HG2 VAL B 143 -22.447 60.987 15.163 1.00 0.00 H ATOM 5020 CA GLU B 144 -16.522 60.650 18.585 1.00 0.25 C ATOM 5022 CA GLU B 144 -15.953 59.324 18.969 1.00 0.25 C ATOM 5025 CB GLU B 144 -15.953 59.324 18.969 1.00 0.25 C ATOM 5026 CG GLU B 144 -17.200 62.889 19.072 1.00 0.25 C ATOM 5028 OE1 GLU B 144 -17.200 62.889 19.072 1.00 0.25 C ATOM 5028 OE1 GLU B 144 -18.626 62.836 19.072 1.00 0.25 C ATOM 5028 OE1 GLU B 144 -18.626 62.836 19.072 1.00 0.25 C ATOM 5028 OE1 GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5030 H GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5031 HA GLU B 144 -18.817 63.075 17.969 1.00 0.00 H ATOM 5033 2HB GLU B 144 -15.773 61.169 17.962 1.00 0.00 H ATOM 5033 2HB GLU B 144 -15.773 61.169 17.962 1.00 0.00 H ATOM 5033 2HB GLU B 144 -15.773 61.169 17.962 1.00 0.00 H ATOM 5037 CA ASP B 145 -16.834 57.030 19.619 1.00 0.22 C ATOM 5039 CA ASP B 145 -16.834 57.331 19.171 1.00 0.22 C ATOM 5030 CA ASP B 145 -16.438 57.030 19.619 1.00 0.22 C ATOM 5030 CA ASP B 145 -16.438 57.030 19.619 1.00 0.22 C C ATOM 5030 CA ASP B 145 -16.438 57.030 19.619 1.00 0.22 C C ATOM 5030 CA ASP B 145 -16.438 57.030 19.619 1.00 0.22 C C ATOM 5030 CA ASP B	35	ATOM ATOM ATOM ATOM	5003 2 5004 3 5005 5006	HG2 THR HG2 THR N VAL CA VAL	B B B B	142 142 143 143	-19.545 -19.002 -20.067 -19.038	58.677 59.711 59.427 59.595	20.799 19.495 16.968 15.985	1.00 1.00 1.00 1.00	0.00 0.00 0.29 0.29	H N C
ATOM 5013 HA VAL B 143 -18.850 58.830 15.329 1.00 0.00 H ATOM 5014 HB VAL B 143 -19.249 61.727 15.730 1.00 0.00 H ATOM 5015 1HG1 VAL B 143 -19.249 61.727 15.730 1.00 0.00 H ATOM 5015 2HG1 VAL B 143 -17.142 61.156 14.609 1.00 0.00 H ATOM 5017 3HG1 VAL B 143 -17.963 59.961 13.575 1.00 0.00 H ATOM 5018 1HG2 VAL B 143 -20.742 61.326 13.578 1.00 0.00 H ATOM 5019 2HG2 VAL B 143 -20.742 61.326 13.578 1.00 0.00 H ATOM 5019 2HG2 VAL B 143 -20.859 59.656 14.667 1.00 0.00 H ATOM 5020 3HG2 VAL B 143 -21.447 60.987 15.163 1.00 0.00 H ATOM 5021 N GLU B 144 -16.522 60.650 18.585 1.00 0.25 N ATOM 5022 CA GLU B 144 -16.522 60.650 18.585 1.00 0.25 N ATOM 5023 C GLU B 144 -16.522 60.650 18.585 1.00 0.25 C ATOM 5023 C GLU B 144 -15.953 59.324 18.969 1.00 0.25 C ATOM 5026 CG GLU B 144 -17.200 62.889 19.597 1.00 0.25 C ATOM 5026 CG GLU B 144 -17.200 62.889 19.597 1.00 0.25 C ATOM 5027 CD GLU B 144 -17.206 62.836 19.072 1.00 0.25 C ATOM 5027 CD GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5028 0E1 GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5029 0E2 GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5031 HA GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5032 1HB GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5033 2HB GLU B 144 -15.773 61.69 17.962 1.00 0.00 H ATOM 5033 1HB GLU B 144 -15.773 61.69 17.962 1.00 0.00 H ATOM 5033 1HB GLU B 144 -15.773 61.461 20.406 1.00 0.00 H ATOM 5033 2HB GLU B 144 -17.460 60.941 20.552 1.00 0.00 H ATOM 5035 2HG GLU B 144 -17.460 60.941 20.552 1.00 0.00 H ATOM 5035 2HG GLU B 144 -17.460 60.941 20.552 1.00 0.00 H ATOM 5037 CA ASP B 145 -16.834 58.331 19.171 1.00 0.22 C ATOM 5037 CA ASP B 145 -16.438 57.030 19.619 1.00 0.22 C ATOM 5037 CA ASP B 145 -16.438 57.030 19.619 1.00 0.22 C ATOM 5037 CA ASP B 145 -16.435 55.797 19.079 1.00 0.22 C ATOM 5030 O ASP B 145 -16.435 55.797 19.079 1.00 0.22 C C ATOM 5030 O ASP B 145 -17.632 56.064 19.718 1.00 0.22 C	40	MOTA MOTA MOTA MOTA	5008 5009 5010 5011	O VAL CB VAL CG1 VAL CG2 VAL	B B B	143 143 143 143	-16.696 -19.256 -18.096 -20.644	59.265 60.803 60.900	16.203 15.127 14.122	1.00 1.00 1.00	0.29 0.29 0.29	0 C C
ATOM 5017 3HG1 VAL B 143 -17.963 59.961 13.559 1.00 0.00 H ATOM 5018 1HG2 VAL B 143 -20.742 61.326 13.578 1.00 0.00 H ATOM 5019 2HG2 VAL B 143 -20.859 59.661 14.167 1.00 0.00 H ATOM 5020 3HG2 VAL B 143 -21.447 60.987 15.163 1.00 0.00 H ATOM 5021 N GLU B 144 -17.728 60.414 17.845 1.00 0.25 N ATOM 5022 CA GLU B 144 -16.522 60.650 18.585 1.00 0.25 C ATOM 5022 C GLU B 144 -16.522 60.650 18.585 1.00 0.25 C ATOM 5024 0 GLU B 144 -16.760 61.452 19.874 1.00 0.25 C ATOM 5025 CB GLU B 144 -16.760 61.452 19.874 1.00 0.25 C ATOM 5026 CG GLU B 144 -16.760 61.452 19.874 1.00 0.25 C ATOM 5027 CD GLU B 144 -18.626 62.836 19.072 1.00 0.25 C ATOM 5028 0E1 GLU B 144 -18.626 62.836 19.072 1.00 0.25 C ATOM 5028 0E1 GLU B 144 -18.626 62.836 19.072 1.00 0.25 C ATOM 5028 0E1 GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5029 0E2 GLU B 144 -18.817 63.075 17.849 1.00 0.25 C ATOM 5031 HA GLU B 144 -18.817 63.075 17.849 1.00 0.25 O ATOM 5033 1HB GLU B 144 -15.773 61.169 17.962 1.00 0.00 H ATOM 5033 1HB GLU B 144 -15.773 61.169 17.962 1.00 0.00 H ATOM 5033 1HB GLU B 144 -15.773 61.169 17.962 1.00 0.00 H ATOM 5033 1HB GLU B 144 -15.773 61.169 17.962 1.00 0.00 H ATOM 5033 1HB GLU B 144 -15.773 61.461 20.406 1.00 0.00 H ATOM 5033 2HB GLU B 144 -16.520 63.373 18.878 1.00 0.00 H ATOM 5035 2HG GLU B 144 -16.520 63.373 18.878 1.00 0.00 H ATOM 5035 2HG GLU B 144 -16.520 63.373 18.878 1.00 0.00 H ATOM 5035 CA ASP B 145 -16.834 58.331 19.171 1.00 0.22 N ATOM 5038 C ASP B 145 -16.834 57.030 19.619 1.00 0.22 C ATOM 5039 0 ASP B 145 -16.438 57.030 19.619 1.00 0.22 C ATOM 5039 0 ASP B 145 -16.438 57.030 19.619 1.00 0.22 C ATOM 5039 0 ASP B 145 -16.438 57.030 19.619 1.00 0.22 C ATOM 5039 0 ASP B 145 -16.438 57.030 19.619 1.00 0.22 C ATOM 5039 0 ASP B 145 -16.438 57.030 19.619 1.00 0.22 C ATOM 5039 0 ASP B 145 -16.439 55.797 19.079 1.00 0.22 C ATOM 5039 0 ASP B 145 -17.632 56.064 19.718 1.00 0.22 C	45	ATOM ATOM ATOM	5013 1 5014 1 5015 11 5016 21	ia val ib val ig1 val ig1 val	B : B : B : B : B : B : B : B : B : B :	143 143 143 143	-18.850 -19.249 -18.282	58.830 61.727 61.693	15.329 15.730 13.377	1.00 1.00 1.00	0.00 0.00 0.00	H H H
ATOM 5022 CA GLU B 144 -16.522 60.650 18.585 1.00 0.25 C ATOM 5023 C GLU B 144 -15.953 59.324 18.969 1.00 0.25 C ATOM 5024 O GLU B 144 -14.738 59.159 19.072 1.00 0.25 C ATOM 5025 CB GLU B 144 -16.760 61.452 19.874 1.00 0.25 C ATOM 5026 CG GLU B 144 -17.200 62.889 19.597 1.00 0.25 C ATOM 5027 CD GLU B 144 -18.626 62.836 19.072 1.00 0.25 C ATOM 5028 OE1 GLU B 144 -19.542 62.548 19.886 1.00 0.25 C ATOM 5029 OE2 GLU B 144 -18.817 63.075 17.849 1.00 0.25 O1-ATOM 5030 H GLU B 144 -18.487 61.065 18.039 1.00 0.00 H ATOM 5031 HA GLU B 144 -15.773 61.169 17.962 1.00 0.00 H ATOM 5032 1HB GLU B 144 -15.773 61.169 17.962 1.00 0.00 H ATOM 5033 2HB GLU B 144 -15.791 61.461 20.406 1.00 0.00 H ATOM 5033 2HB GLU B 144 -17.460 60.941 20.552 1.00 0.00 H ATOM 5035 2HG GLU B 144 -17.460 60.941 20.552 1.00 0.00 H ATOM 5035 2HG GLU B 144 -17.181 63.464 20.537 1.00 0.00 H ATOM 5035 2HG GLU B 144 -17.181 63.464 20.537 1.00 0.00 H ATOM 5037 CA ASP B 145 -16.834 58.331 19.171 1.00 0.22 C ATOM 5038 C ASP B 145 -16.834 58.331 19.171 1.00 0.22 C ATOM 5039 O ASP B 145 -16.488 57.030 19.619 1.00 0.22 C ATOM 5039 O ASP B 145 -15.451 56.448 18.657 1.00 0.22 C ATOM 5039 C BASP B 145 -15.451 56.448 18.657 1.00 0.22 C	50	ATOM ATOM ATOM	5018 1E 5019 2E 5020 3E	IG2 VAL IG2 VAL IG2 VAL	B 1 B 1	143 143 143	-20.742 -20.859 -21.447	59.961 61.326 59.656 60.987	13.559 13.578 14.167 15.163	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
ATOM 5028 OE1 GLU B 144 -19.542 62.548 19.886 1.00 0.25 O ATOM 5029 OE2 GLU B 144 -18.817 63.075 17.849 1.00 0.25 O1- ATOM 5030 H GLU B 144 -18.487 61.065 18.039 1.00 0.00 H ATOM 5031 HA GLU B 144 -15.773 61.169 17.962 1.00 0.00 H ATOM 5032 1HB GLU B 144 -15.791 61.461 20.406 1.00 0.00 H ATOM 5033 2HB GLU B 144 -17.460 60.941 20.552 1.00 0.00 H ATOM 5034 1HG GLU B 144 -17.460 60.941 20.552 1.00 0.00 H ATOM 5035 2HG GLU B 144 -17.181 63.464 20.537 1.00 0.00 H ATOM 5036 N ASP B 145 -16.834 58.331 19.171 1.00 0.22 N ATOM 5037 CA ASP B 145 -16.438 57.030 19.619 1.00 0.22 C ATOM 5039 O ASP B 145 -15.451 56.448 18.657 1.00 0.22 C ATOM 5039 O ASP B 145 -14.495 55.797 19.079 1.00 0.22 C	55	ATOM ATOM ATOM ATOM ATOM	5022 C 5023 C 5024 C 5025 C 5026 C	CA GLU CB GLU CB GLU CB GLU	B 1 B 1 B 1 B 1	144 144 144 144	-16.522 -15.953 -14.738 -16.760 -17.200	60.650 59.324 59.159 61.452	18.585 18.969 19.072 19.874	1.00 1.00 1.00 1.00	0.25 0.25 0.25 0.25	С С С
ATOM 5033 2HB GLU B 144 -17.460 60.941 20.552 1.00 0.00 H ATOM 5034 1HG GLU B 144 -16.520 63.373 18.878 1.00 0.00 H ATOM 5035 2HG GLU B 144 -17.181 63.464 20.537 1.00 0.00 H ATOM 5036 N ASP B 145 -16.834 58.331 19.171 1.00 0.22 N ATOM 5037 CA ASP B 145 -16.438 57.030 19.619 1.00 0.22 C ATOM 5038 C ASP B 145 -15.451 56.448 18.657 1.00 0.22 C ATOM 5039 O ASP B 145 -14.495 55.797 19.079 1.00 0.22 C ATOM 5040 CB ASP B 145 -17.632 56.064 19.718 1.00 0.22 C	60	ATOM ATOM ATOM ATOM	5028 C 5029 C 5030 H 5031 H	E1 GLU E2 GLU GLU A GLU	B 1 B 1 B 1 B 1	44 44 44 44	-19.542 -18.817 -18.487 -15.773	62.548 63.075 61.065 61.169	19.886 17.849 18.039	1.00 1.00 1.00	0.25 0.25 0.00	0 01- H
ATOM 5037 CA ASP B 145 -16.438 57.030 19.619 1.00 0.22 C ATOM 5038 C ASP B 145 -15.451 56.448 18.657 1.00 0.22 C ATOM 5039 O ASP B 145 -14.495 55.797 19.079 1.00 0.22 O ATOM 5040 CB ASP B 145 -17.632 56.064 19.718 1.00 0.22 C	65	ATOM ATOM ATOM ATOM	5033 2H 5034 1H 5035 2H 5036 N	B GLU G GLU G GLU ASP	B 1 B 1 B 1 B 1	44 44 44 45	-17.460 -16.520 -17.181	60.941 63.373 63.464	20.552 18.878 20.537	1.00 1.00 1.00	0.00 0.00 0.00	H H H H
	70	ATOM ATOM ATOM	5038 C 5039 O 5040 C	ASP ASP B ASP	B 1-B 1-B 1-B	45 45 45 45	-16.438 -15.451 -14.495 -17.632	57.030 56.448 55.797 56.064	19.619 18.657 19.079 19.718	1.00 1.00 1.00 1.00	0.22 0.22 0.22 0.22	с с о с

	ATOM	5042 O	D1 ASP B 145	-16.20	1 54.160	19.992	1.00	0.22	0
	ATOM		02 ASP B 145						01-
	MOTA	5044 H	ASP B 145						н
5	ATOM				0 57.121			0.00	Н
5	ATOM					18.717	1.00	0.00	н
	MOTA					20.264		0.00	H
	ATOM ATOM		SER B 146					0.20	N
	ATOM							0.20	С
10	MOTA	5051 0	SER B 146 SER B 146					0.20	С
	ATOM	5052 CI						0.20	0
	ATOM	5053 00						0.20	C
	ATOM	5054 н	SER B 146					0.20	0
	ATOM	5055 HZ					1.00	0.00	H
15	MOTA	5056 1HE				14.651	1.00	0.00	H H
	MOTA	5057 2HB					1.00	0.00	H
	ATOM	5058 HG	SER B 146	-15.343			1.00	0.00	H
	ATOM	5059 N	GLY B 147	-12.394		16.442	1.00	0.21	N
0.0	MOTA	5060 CA		-11.020		16.735	1.00	0.21	c
20	ATOM	5061 C	GLY B 147	-10.301		16.762	1.00	0.21	č
	ATOM	5062 O	GLY B 147	-10.814	53.517	16.299	1.00	0.21	ŏ
	MOTA	5063 н	GLY B 147	-12.613	54.654	16.041	1.00	0.00	H
	ATOM	5064 1HA		-10.942		17.716	1.00	0.00	H
25	ATOM	5065 2HA		-10.567		15.975	1.00	0.00	H
23	ATOM ATOM	5066 N	THR B 148	-9.071		17.306	1.00	0.17	N
	ATOM	5067 CA 5068 C		-8.323		17.360	1.00	0.17	C
	ATOM	5068 C 5069 O	THR B 148 THR B 148	-8.332		18.779	1.00	0.17	С
	ATOM	5070 CB	THR B 148	-8.106		19.694	1.00	0.17	0
30	ATOM		1 THR B 148	-6.895 -6.829		16.948	1.00	0.17	C
	ATOM	5072 CG		-6.209	53.999 52.120	15.623	1.00	0.17	0
	ATOM	5073 H	THR B 148	-8.624	55.388	17.013 17.678	1.00	0.17	C
	ATOM	5074 HA	THR B 148	-8.767	52.588	16.674	1.00	0.00	H
	ATOM	5075 HB	THR B 148	-6.364	54.181	17.632	1.00	0.00	H H
35	ATOM	5076 HG	L THR B 148	-7.244	54.874	15.660	1.00	0.00	H
	ATOM	5077 1HG	THR B 148	-5.147	52.241	16.751	1.00	0.00	H
	MOTA	5078 2HG	THR B 148	-6.308	51.719	18.025	1.00	0.00	н
	ATOM		THR B 148	-6.655	51.422	16.289	1.00	0.00	Н
40	MOTA	5080 N	TYR B 149	-8.616	51.574	19.001	1.00	0.12	N
40	ATOM	5081 CA	TYR B 149	-8.660	51.076	20.343	1.00	0.12	С
	ATOM	5082 C	TYR B 149	-7.643	49.994	20.494	1.00	0.12	С
	ATOM	5083 O	TYR B 149	-7.419	49.197	19.586	1.00	0.12	0
	ATOM ATOM	5084 CB 5085 CG	TYR B 149	-9.999	50.428	20.732	1.00	0.12	С
45	ATOM		TYR B 149 TYR B 149	-11.045	51.479	20.866	1.00	0.12	С
10	ATOM		TYR B 149	-11.674	51.998	19.759	1.00	0.12	С
	ATOM		TYR B 149	-11.402	51.932	22.113	1.00	0.12	C
	ATOM	5089 CE2		-12.644 -12.372	52.962	19.899	1.00	0.12	C
	ATOM	5090 CZ	TYR B 149	-12.993	52.895	22.260	1.00	0.12	C
50	ATOM	5091 OH	TYR B 149	-13.989	53.412 54.400	21.150	1.00	0.12	C
	ATOM	5092 н	TYR B 149	-8.796	50.923	21.293 18.245	1.00 1.00	0.12	o H
	ATOM	5093 HA	TYR B 149	-8.441	51.899	21.010		0.00	n H
	ATOM	5094 1HB	TYR B 149	-9.845	49.950	21.708	1.00	0.00	H
	ATOM	5095 2HB	TYR B 149	-10.289	49.654	20.005	1.00	0.00	н
55	ATOM	5096 HD1	TYR B 149	-11.402	51.655	18.764	1.00	0.00	H
	MOTA		TYR B 149	-10.961	51.469	22.992	1.00	0.00	н
	MOTA		TYR B 149	-13.123	53.373	19.011	1.00	0.00	H
	MOTA		TYR B 149	-13.003	52.773	23.120	1.00	0.00	н
60	ATOM	5100 HH	TYR B 149	-14.641	54.316	20.555		0.00	H
60	ATOM	5101 N	TYR B 150	-6.980	49.968	21.666		0.12	N
	ATOM	5102 CA	TYR B 150	-6.072	48.906	21.976	1.00	0.12	С
	ATOM	5103 C	TYR B 150	-6.183	48.678	23.446	1.00	0.12	С
	ATOM	5104 0	TYR B 150	-6.750	49.497	24.169	1.00	0.12	0
65	ATOM	5105 CB	TYR B 150	-4.574	49.181	21.581		0.12	С
0.5	ATOM	5106 CG	TYR B 150	-4.087	50.632	21.583		0.12	С
	ATOM		TYR B 150	-2.898	50.942	22.234		0.12	С
	MOTA MOTA		TYR B 150	-4.656	51.650			0.12	C
	ATOM		TYR B 150 TYR B 150	-2.277	52.174			0.12	C
70	MOTA	5110 CE2	TYR B 150	-4.087 -2.865	52.909			0.12	C
	ATOM	5111 CZ 5112 OH	TYR B 150	-2.865 -2.303				0.12	C
				2.303	~ 3 . 3 1 /	44.411	1.00 (0.12	0

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5118 H 5119 H	B TYR B 150	-7.179 -6.417 -4.376 -3.930 -2.411 -5.552	47.983 48.771 48.575 50.183 51.456 52.306	21.478 20.583 22.238 22.843 20.231 22.582	1.00 1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00 0.00	н н н н н
10	ATOM ATOM ATOM ATOM ATOM	5121 HF 5122 N 5123 CF 5124 C 5125 O	TYR B 150 CYS B 151	-4.566 -1.388 -5.668 -5.851 -4.536	53.669 54.382 47.538 47.259 46.869 46.384	21.485 23.936 25.325 25.912	1.00 1.00 1.00 1.00	0.00 0.00 0.27 0.27 0.27	H N C
15	ATOM ATOM ATOM ATOM ATOM	5126 CF 5127 SG 5128 H 5129 H2 5130 1HE	CYS B 151 CYS B 151 CYS B 151 CYS B 151	-6.843 -7.171 -5.059 -6.218 -6.499	46.104 45.727 46.930 48.148 45.191	25.215 25.548 27.291 23.420 25.849 25.037	1.00 1.00 1.00 1.00	0.27 0.27 0.27 0.00 0.00	О S Н Н
20	MOTA MOTA ATOM MOTA MOTA	5131 2HE 5132 N 5133 CA 5134 C 5135 O	CYS B 151 THR B 152	-7.796 -4.373 -3.202 -3.659 -4.747	46.404 47.128 46.713 45.920 46.133	25.083 27.222 27.934 29.104 29.635	1.00 1.00 1.00 1.00	0.00 0.37 0.37 0.37	H N C
25	ATOM ATOM ATOM MOTA MOTA	5136 CB	THR B 152 1 THR B 152 2 THR B 152 THR B 152	-2.327 -3.105 -1.524 -5.082 -2.623	47.824 48.812 48.412 47.588	28.434 29.091 27.271 27.778	1.00 1.00 1.00 1.00	0.37 0.37 0.37 0.37 0.00	о с н
30	ATOM ATOM ATOM ATOM ATOM	5141 HB	THR B 152 1 THR B 152 2 THR B 152 2 THR B 152	-2.623 -1.602 -2.553 -0.892 -0.852 -2.185	46.045 47.395 49.611 49.248 47.655 48.790	27.283 29.156 29.152 27.611 26.850	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
35	ATOM ATOM ATOM ATOM ATOM	5146 N 5147 CA 5148 C 5149 O 5150 H	GLY B 153 GLY B 153 GLY B 153 GLY B 153	-2.829 -3.195 -1.974 -1.021	44.947 44.136 43.392 43.278	26.476 29.520 30.637 31.040 30.271	1.00 1.00 1.00 1.00	0.00 0.21 0.21 0.21 0.21	н С С О
40	ATOM ATOM ATOM ATOM ATOM	5151 1HA 5152 2HA 5153 N 5154 CA 5155 C	GLY B 153 GLY B 153 GLY B 153 LYS B 154 LYS B 154	-1.886 -3.993 -3.543 -1.972 -0.807	44.837 43.422 44.766 42.860 42.155	29.146 30.370 31.450 32.275 32.702	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.12 0.12	H H N C
45	ATOM ATOM ATOM ATOM	5156 O 5157 CB 5158 CG 5159 CD	LYS B 154 LYS B 154 LYS B 154 LYS B 154 LYS B 154	-1.155 -2.059 -0.290 0.176 0.395	40.715 40.336 42.601 44.056 44.591	32.821 33.565 34.077 34.106 35.521	1.00 1.00 1.00 1.00	0.12 0.12 0.12 0.12 0.12	00000
50	ATOM ATOM ATOM ATOM ATOM	5160 CE 5161 NZ 5162 H 5163 HA 5164 1HB	LYS B 154 LYS B 154 LYS B 154 LYS B 154 LYS B 154	0.863 1.046 -2.733 -0.031 0.526	46.048 46.488 42.972 42.235 41.927	35.557 36.959 32.935 31.958 34.362	1.00 1.00 1.00 1.00	0.12 0.12 0.00 0.00	C N1+ H H
55	MOTA ATOM ATOM ATOM ATOM MOTA MOTA	5165 2HB 5166 1HG 5167 2HG 5168 1HD 5169 2HD 5170 1HE	LYS B 154 LYS B 154 LYS B 154 LYS B 154 LYS B 154 LYS B 154 LYS B 154	-1.176 -0.548 1.115 1.072 -0.602	42.511 44.710 44.114 43.927 44.565	34.684 33.586 33.543 36.083 35.950	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	н н н н
60	ATOM ATOM ATOM ATOM ATOM	5171 2HE 5172 1HZ 5173 2HZ 5174 3HZ 5175 N	LYS B 154 LYS B 154 LYS B 154 LYS B 154 LYS B 154 VAL B 155	0.129 1.829 1.435 0.179 1.701	46.719 46.180 47.422 46.508 45.889	35.080 35.041 36.999 37.465 37.446	1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00	H H H H
65	ATOM ATOM ATOM ATOM ATOM	5176 CA 5177 C 5178 O 5179 CB	VAL B 155 VAL B 155 VAL B 155 VAL B 155 VAL B 155	-0.620 0.646 1.735 -0.804	39.872 38.462 37.984 38.387 37.761	32.056 32.171 32.782 32.374 30.854		0.20 0.20 0.20 0.20 0.20	N C C C
70	ATOM ATOM ATOM		VAL B 155 VAL B 155 VAL B 155 VAL B 155	0.465	40.165	30.221 29.983 31.706 32.829	1.00 1.00	0.20 0.20 0.00 0.00	С Н Н

	ATOM ATOM		3 VAL B 155	-0.898 -2.526				0.00	H H
	ATOM		1 VAL B 155	-2.861				0.00	H
r	MOTA		1 VAL B 155	-1.975				0.00	н
5	ATOM		2 VAL B 155	0.249				0.00	H
	MOTA MOTA		2 VAL B 155	0.649				0.00	H
	ATOM	5190 3HG	2 VAL B 155 TRP B 156	1.343 0.539		30.285		0.00	H
	ATOM	5192 CA		1.740	36.713			0.33	N C
10	ATOM	5193 C	TRP B 156	2.323	37.955			0.33	c
	ATOM	5194 0	TRP B 156	1.605	38.904			0.33	Ö
	MOTA	5195 CB		2.765	36.100	33.483	1.00	0.33	С
	ATOM ATOM	5196 CG 5197 CD		2.277	34.858			0.33	С
15	ATOM		1 TRP B 156 2 TRP B 156	1.694 2.345	34.753 33.525			0.33	C
	ATOM		1 TRP B 156	1.392	33.439	33.303 31.275	1.00	0.33 0.33	C
	ATOM	5200 CE	2 TRP B 156	1.787	32.671	32.350	1.00	0.33	N C
	ATOM		3 TRP B 156	2.832	33.050	34.487	1.00	0.33	č
20	ATOM	5202 CZ		1.705	31.325	32.569	1.00	0.33	С
20	MOTA MOTA		3 TRP B 156 2 TRP B 156	2.748	31.691	34.703	1.00	0.33	С
	ATOM	5204 CH	TRP B 156	2.195 -0.349	30.845 36.804	33.763 34.155	1.00	0.33	C
	ATOM	5206 HA	TRP B 156	1.505	36.007	34.133	1.00 1.00	0.00	H H
	MOTA	5207 1HB	TRP B 156	3.617	35.752	34.092	1.00	0.00	H
25	MOTA	5208 2HB	TRP B 156	3.230	36.786	32.765	1.00	0.00	H
	MOTA		1 TRP B 156	1.470	35.527	30.827	1.00	0.00	H
	ATOM ATOM	5210 HE3	TRP B 156	0.852 3.265	33.107	30.508	1.00	0.00	H
	ATOM		TRP B 156	1.272	33.702 30.662	35.237 31.826	1.00 1.00	0.00 0.00	H H
30	ATOM	5213 HZ3		3.122	31.273	35.635	1.00	0.00	H
	ATOM		TRP B 156	2.143	29.779	33.972	1.00	0.00	н
	MOTA	5215 N	GLN B 157	3.656	37.967	35.190	1.00	0.49	N
	ATOM ATOM	5216 CA	GLN B 157	4.338	39.097	35.739	1.00	0.49	С
35	ATOM	5217 C 5218 O	GLN B 157 GLN B 157	4.276 4.048	40.236	34.773	1.00	0.49	С
	ATOM	5219 CB	GLN B 157	5.830	41.381 38.816	35.160 35.969	1.00 1.00	0.49 0.49	0
	ATOM	5220 CG	GLN B 157	6.082	37.569	36.814	1.00	0.49	C
	ATOM	5221 CD	GLN B 157	5.294	37.721	38.101	1.00	0.49	č
40	ATOM		GLN B 157	5.354	38.759	38.756	1.00	0.49	0
40	ATOM ATOM	5223 NE2 5224 H	GLN B 157 GLN B 157	4.525	36.663	38.466	1.00	0.49	N
	ATOM	5225 HA	GLN B 157	4.224 3.849	37.178 39.413	34.941 36.673	1.00 1.00	0.00	H
	ATOM	5226 1HB	GLN B 157	6.280	39.706	36.442	1.00	0.00	H H
4 =	MOTA	5227 2HB	GLN B 157	6.355	38.651	35.031	1.00	0.00	H
45	ATOM	5228 1HG	GLN B 157	7.147	37.485	37.094	1.00	0.00	H
	ATOM ATOM	5229 2HG 5230 1HE2	GLN B 157	5.821	36.652	36.260	1.00	0.00	H
	ATOM	5231 2HE2		4.495 3.997	35.810 36.763	37.942	1.00	0.00	H
	ATOM	5232 N	LEU B 158	4.459	39.934	39.316 33.473	1.00	0.00	H N
50	ATOM	5233 CA	LEU B 158	4.607	40.961	32.483	1.00	0.41	C
	ATOM	5234 C	LEU B 158	3.306	41.597	32.127	1.00	0.41	č
	ATOM	5235 O	LEU B 158	2.227	41.063	32.381	1.00	0.41	0
	ATOM ATOM	5236 CB 5237 CG	LEU B 158 LEU B 158	5.252	40.467	31.176	1.00	0.41	C
55	ATOM		LEU B 158	6.699 7.628	39.977 41.124	31.364 31.796	1.00	0.41	C
	ATOM		LEU B 158	6.758	38.765	32.310	1.00	0.41	C C
	ATOM	5240 H	LEU B 158	4.371	38.990	33.144	1.00	0.00	н
	ATOM	5241 HA	LEU B 158	5.247	41.746	32.926		0.00	н
60	MOTA	5242 1HB	LEU B 158	5.231	41.276	30.425		0.00	H
00	ATOM ATOM	5243 2HB 5244 HG	LEU B 158 LEU B 158	4.656	39.640	30.773		0.00	H
	ATOM	5244 HG 5245 1HD1		7.047 8.682	39.639 40.800	30.367		0.00	H
	ATOM	5246 2HD1	LEU B 158	7.548	41.983	31.788 31.109		0.00 0.00	H H
	ATOM	5247 3HD1	LEU B 158	7.408	41.481	32.814		0.00	n H
65	ATOM	5248 1HD2	LEU B 158	7.652	38.158	32.086		0.00	Н
	MOTA	5249 2HD2		_	39.116	33.331	-	0.00	Н
	MOTA	5250 3HD2			38.090	32.222		0.00	H
	ATOM ATOM		ASP B 159 ASP B 159			31.533		0.19	N
70	ATOM		ASP B 159			31.058 29.566		0.19 0.19	C
	ATOM		ASP B 159			29.009		0.19	С 0
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	ATOM ATOM ATOM	5255 CI 5256 CC 5257 OI		2.381 1.124 0.378	45.839	31.117	1.00	0.19	C
5	ATOM ATOM ATOM		D2 ASP B 159 ASP B 159	0.904 4.304 1.394	46.910	30.205 31.744 31.275 31.412	1.00	0.19 0.19 0.00	0 01- H
	MOTA MOTA	5261 1HI 5262 2HI 5263 N	ASP B 159	3.242 2.576 1.279	45.547	31.017 32.581 28.874	1.00	0.00 0.00 0.00 0.11	H H H
10	ATOM ATOM ATOM	5264 CZ 5265 C 5266 O		1.321 0.381 -0.535	43.282 44.304 44.755	27.443 26.901 27.589	1.00 1.00	0.11 0.11 0.11	N C C
15	ATOM ATOM ATOM	5267 CE 5268 CG	TYR B 160	0.884 1.939 2.067	41.929 40.924 40.404	26.857 27.171 28.439	1.00	0.11 0.11 0.11	000
	MOTA MOTA MOTA	5271 CE 5272 CE	22 TYR B 160 31 TYR B 160 32 TYR B 160	2.794 3.042 3.771	40.488 39.476 39.560	26.185 28.720 26.459	1.00 1.00 1.00	0.11 0.11 0.11	000
20	ATOM ATOM ATOM	5273 C2 5274 OH 5275 H	TYR B 160 TYR B 160	3.895 4.895 0.420	39.052 38.099 43.679	27.730 28.019 29.317	1.00 1.00 1.00	0.11 0.11 0.00	С О Н
25	ATOM ATOM ATOM ATOM	5276 HA 5277 1HB 5278 2HB	TYR B 160 TYR B 160	2.324 0.755 -0.098	43.539 42.037 41.635	27.087 25.769 27.262	1.00 1.00 1.00	0.00 0.00 0.00	н н н
23	ATOM ATOM ATOM	5280 HD 5281 HE	1 TYR B 160 2 TYR B 160 1 TYR B 160 2 TYR B 160	1.419 2.708 3.087 4.440	40.777 40.890 39.038 39.242	29.225 25.178 29.711	1.00 1.00 1.00	0.00 0.00	H H H
30	MOTA MOTA MOTA	5283 HH 5284 N 5285 CA	TYR B 160 GLU B 161	5.695 0.622 -0.262	38.392 44.722 45.647	25.662 27.561 25.643 25.000	1.00 1.00 1.00 1.00	0.00 0.00 0.12 0.12	H H N C
0.5	ATOM ATOM ATOM	5286 C 5287 O 5288 CB	GLU B 161 GLU B 161 GLU B 161	-0.753 -0.033 0.273	44.973 44.197 47.006	23.762 23.135 24.485	1.00 1.00 1.00	0.12 0.12 0.12	000
35	ATOM ATOM ATOM		GLU B 161 GLU B 161 1 GLU B 161	-0.616 0.100 0.523	48.163 48.894 48.163	23.930 22.732 21.832	1.00 1.00 1.00	0.12 0.12 0.12	с с о
40	MOTA MOTA MOTA	5292 OE 5293 H 5294 HA 5295 1HB	GLU B 161 GLU B 161 GLU B 161	0.153 1.327 -1.119	50.124 44.317 45.827	22.811 25.048 25.660	1.00 1.00 1.00	0.12 0.00 0.00	01- Н Н
	MOTA MOTA MOTA	5296 2HB 5296 2HB 5297 1HG 5298 2HG	GLU B 161 GLU B 161 GLU B 161 GLU B 161	0.959 0.855 -0.844 -1.583	46.729 47.435 48.899 47.807	23.673 25.316 24.714	1.00 1.00 1.00	0.00	H H H
45	ATOM ATOM ATOM	5299 N 5300 CA 5301 C	SER B 162 SER B 162 SER B 162	-2.020 -2.598 -2.381	45.234 44.616 45.499	23.551 23.397 22.242 21.065	1.00 1.00 1.00	0.00 0.11 0.11 0.11	H C C
50	MOTA MOTA MOTA	5302 O 5303 CB 5304 OG	SER B 162 SER B 162 SER B 162	-1.967 -4.113 -4.614	46.650 44.377 43.756	21.196 22.371 21.196	1.00 1.00 1.00	0.11 0.11 0.11	0 C O
	ATOM ATOM ATOM	5305 H 5306 HA 5307 1HB	SER B 162 SER B 162 SER B 162	-2.583 -2.119 -4.658	45.884 43.636 45.313	23.935 22.074 22.560	1.00	0.00	H H H
55	ATOM ATOM ATOM	5308 2HB 5309 HG 5310 N	SER B 162 SER B 162 GLU B 163	-4.320 -4.572 -2.640	43.696 44.455 44.951	23.199 20.511 19.864	1.00 1.00 1.00	0.00 0.00 0.13	H H N
60	ATOM ATOM ATOM ATOM	5311 CA 5312 C 5313 O 5314 CB	GLU B 163 GLU B 163 GLU B 163 GLU B 163	-2.517 -3.757 -4.830	45.715 46.533 46.148	18.661 18.544 19.006	1.00 1.00 1.00	0.13 0.13 0.13	C C O
	ATOM ATOM ATOM	5315 CG 5316 CD	GLU B 163 GLU B 163 GLU B 163	-2.382 -3.567 -3.153 -2.076	44.835 43.890 42.846 42.223	17.407 17.202 16.177 16.381	1.00 1.00 1.00 1.00	0.13 0.13 0.13 0.13	0000
65	ATOM ATOM ATOM		GLU B 163 GLU B 163 GLU B 163	-3.900 -2.775 -1.567	42.654 43.955 46.269	15.181 19.742 18.725	1.00 1.00 1.00	0.13 0.00 0.00	01- Н Н
	ATOM ATOM ATOM	5321 1HB 5322 2HB 5323 1HG	GLU B 163 GLU B 163 GLU B 163	-1.436 -2.268 -4.480	44.272 45.510 44.422	17.498 16.541 16.897	1.00 1.00	0.00 0.00 0.00	H H H
70	MOTA MOTA	5324 2HG 5325 N	GLU B 163 PRO B 164	-3.770 -3.611	43.349 47.681	18.136 17.956	1.00	0.00	H N

	ATOM ATOM	5326 5327		PRO PRO	B 164 B 164				1.00	0.13 0.13	c c
	MOTA	5328	0	PRO	B 164	-5.235	47.407		1.00	0.13	ŏ
5	MOTA	5329		PRO				17.565	1.00	0.13	С
J	MOTA MOTA	5330 5331			B 164 B 164			18.251	1.00	0.13	C
	MOTA	5332			B 164			18.167 18.778	1.00	0.13	C H
	MOTA		1HB		B 164			18.086	1.00	0.00	H
1.0	ATOM		2HB		B 164		50.174	16.494	1.00	0.00	н
10	ATOM		1HG		B 164		50.209	19.302	1.00	0.00	H
	MOTA MOTA		2HG 1HD		B 164 B 164			17.804	1.00	0.00	H
	ATOM	5338			B 164	-1.699 -1.875	48.263 48.165	17.323 19.100	1.00	0.00	H H
	ATOM	5339			B 165	-6.982	48.383	16.888	1.00	0.11	N
15	MOTA	5340			B 165	-7.932	48.026	15.879	1.00	0.11	c
	MOTA	5341			B 165	-8.678	49.279	15.565	1.00	0.11	C
	ATOM ATOM	5342 5343			B 165 B 165	-8.896 -8.953	50.112	16.444	1.00	0.11	0
	ATOM	5344			B 165	-8.309	46.969 45.618	16.327 16.688	1.00	0.11	C
20	ATOM	5345		LEU		-9.377	44.562	17.011	1.00	0.11	Ċ
	ATOM	5346	CD2	LEU	в 165	-7.321	45.158	15.605	1.00	0.11	č
	ATOM	5347	H		B 165	-7.332	48.855	17.713	1.00	0.00	Ħ
	MOTA	5348	HA		B 165	-7.399	47.693	14.975	1.00	0.00	H
25	ATOM ATOM	5349 5350			B 165 B 165	-9.663 -9.540	46.827 47.354	15.492 17.180	1.00	0.00	H
20	ATOM	5351	HG		B 165	-7.725	45.756	17.180	1.00	0.00	H H
	ATOM			LEU		-8.889	43.616	17.270	1.00	0.00	H
	ATOM			LEU		-10.014	44.907	17.841	1.00	0.00	н
30	ATOM			LEU 1		-10.046	44.410	16.150	1.00	0.00	H
30	MOTA MOTA			LEU I		-7.258 -7.617	44.060	15.620	1.00	0.00	H
	ATOM			LEU		-7.617 -6.293	45.460 45.461	14.591 15.796	1.00 1.00	0.00	H H
	ATOM	5358	N		B 166	-9.077	49.464	14.294	1.00	0.10	N
	MOTA	5359	CA	ASN I		-9.772	50.674	13.976	1.00	0.10	č
35	ATOM	5360	С		3 166	-11.234	50.388	14.008	1.00	0.10	С
	MOTA	5361	O	ASN I		-11.729	49.520	13.291	1.00	0.10	0
	MOTA ATOM	5362 5363	CB CG	ASN I		-9.460 -8.056	51.243 51.831	12.581 12.593	$1.00 \\ 1.00$	0.10 0.10	C
	ATOM	5364		ASN I		-7.304	51.681	13.555	1.00	0.10	o
40	ATOM	5365		ASN I		-7.695	52.538	11.490	1.00	0.10	N
	ATOM	5366	H	ASN I		-8.920	48.814	13.545	1.00	0.00	H
	atom atom	5367 5368	HA	ASN E		-9.511	51.470	14.693	1.00	0.00	H
	ATOM	5369	2HB	ASN E		-10.185 -9. 55 5	52.051 50.487	12.379 11.785	1.00 1.00	0.00	H H
45	ATOM			ASN E		-8.314	52.676	10.714	1.00	0.00	н
	ATOM	5371	2HD2	ASN E	166	-6.780	52.955	11.511	1.00	0.00	H
	ATOM	5372	N	ILE E		-11.959	51.119	14.873	1.00	0.22	N
	ATOM ATOM	5373 5374	CA C	ILE E		-13.378 -13.954	50.962	14.942	1.00	0.22	C
50	ATOM	5375	Ö	ILE E		-13.535	52.275 53.322	14.545 15.035	1.00	0.22 0.22	С 0
	ATOM	5376	СВ	ILE E		-13.880	50.650	16.322	1.00	0.22	č
	ATOM	5377	CG1	ILE B	167	-13.316	49.304				С
	ATOM	5378		ILE B		-15.418	50.705	16.294	1.00	0.22	С
55	ATOM ATOM	5379		ILE B		-13.532	49.051	18.297	1.00	0.22	C
55	ATOM	5380 5381	H HA	ILE B		-11.568 -13.699	51.8 84 50.161	15.416 14.261	1.00	0.00	H H
	ATOM	5382	HB	ILE B		-13.530	51.440	17.014	1.00	0.00	H
	MOTA	5383	1HG1	ILE B	167	-12.227	49.256	16.623	1.00	0.00	H
CO	MOTA			ILE B		-13.758	48.478	16.219	1.00	0.00	H
60	MOTA			ILE B		-15.829	50.544	17.306	1.00	0.00	H
	ATOM ATOM			ILE B		-15.817 -15.851	51.680 49.914	15.976	1.00	0.00	H
	ATOM			ILE B		-13.851	49.914	15.670 18.621	1.00 1.00	0.00	H H
	ATOM			ILE B		-13.158	49.884	18.909	1.00	0.00	H
65	MOTA	5390		ILE B	167	-14.602	48.923	18.511	1.00	0.00	н
	ATOM	5391	N	THR B		-14.926	52.262	13.618	1.00	0.48	N
	ATOM	5392	CA	THR B		-15.488	53.513	13.212	1.00	0.48	C
	ATOM ATOM	5393 5394	С 0	THR B		-16.955 -17.587	53.470 52.419	13.410 13.312	1.00	0.48	С 0
70	ATOM	5395	СВ	THR B		-15.289	53.846	11.764	1.00	0.48	c
	ATOM	5396		THR B		-15.798	52.802	10.948	1.00	0.48	ŏ

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ATOM 5397 CG2 THR B 168 -13.800 54.078 11.494 1.00 0.48 C ATOM 5398 H THR B 168 -15.33351.415 13.242 1.00 0.00 Н ATOM 5399 HA THR B 168 -15.086 54.315 13.823 1.00 0.00 н 5400 ATOM HB THR B 168 -15.828 54.788 11.542 1.00 0.00 Н 5 -16.752 -13.629 ATOM 5401 HG1 THR B 168 52.753 11.109 1.00 0.00 ATOM 5402 1HG2 THR B 168 54.378 10.447 1.00 0.00 Н MOTA 5403 2HG2 THR B 168 -13.392 54.871 12.141 1.00 0.00 H MOTA 5404 3HG2 THR B 168 -13.218 53.159 11.670 1.00 0.00 H MOTA 5405 N **VAL B 169** -17.538 54.638 13.724 1.00 0.55 N 10 ATOM 5406 CA **VAL B 169** -18.958 54.667 13.795 1.00 0.55 C ATOM 5407 С VAL B 169 -19.375 55.038 12.415 1.00 0.55 C ATOM 5408 VAL B 169 O -18.935 56.046 11.863 1.00 0.55 0 ATOM 5409 CB **VAL B 169** -19.532 55.659 14.771 1.00 0.55 ATOM 5410 CG1 VAL B 169 -19.096 55.245 16.183 1.00 0.55 C 15 CG2 VAL B 169 MOTA 5411 -19.102 57.084 14.391 1.00 0.55 C MOTA 5412 **VAL** B 169 -17.097 Ħ 55.537 13.643 1.00 0.00 Н ATOM 5413 HA **VAL B 169** -19.344 53.676 14.069 1.00 0.00 H ATOM 5414 HB **VAL B 169** -20.631 55.570 14.679 1.00 0.00 MOTA 5415 1HG1 VAL B 169 -19.882 55.434 16.925 1.00 0.00 H 20 ATOM 5416 2HG1 VAL B 169 -18.919 54.158 16.250 1.00 0.00 H ATOM 5417 3HG1 VAL B 169 -18.150 55.715 16.482 1.00 0.00 H MOTA 5418 1HG2 VAL B 169 -19.962 57.610 14.838 1.00 0.00 H MOTA 5419 2HG2 VAL B 169 -18.107 57.258 14.822 1.00 0.00 H ATOM 5420 3HG2 VAL B 169 -19.091 57.488 13.385 1.00 0.00 H 25 MOTA 5421 ILE B 170 N -20.221 54.194 11.807 1.00 0.56 N ATOM 5422 54.415 55.721 CA **ILE B 170** -20.637 10.457 1.00 0.56 C ATOM 5423 С **ILE B 170** -21.357 10.428 1.00 0.56 C ILE B 170 ILE B 170 MOTA 5424 0 -21.198 56.502 9.490 1.00 0.56 0 ATOM 5425 CB -21.546 53.321 9.942 1.00 0.56 C 30 MOTA 5426 CG1 ILE B 170 -21.728 53.399 8.414 1.00 0.56 ATOM 5427 CG2 ILE B 170 -22.867 53.374 10.727 1.00 0.56 C ATOM CD1 ILE B 170 5428 -22.467 54.643 7.921 1.00 0.56 C MOTA 5429 ILE B 170 H -20.615 53.381 12,272 1.00 0.00 H ATOM 5430 HA ILE B 170 -19.739 54.517 9.824 1.00 0.00 35 -21.142 MOTA 5431 HB **ILE B 170** 52.353 10.164 1.00 0.00 H ATOM 5432 1HG1 ILE B 170 -22.296 52.506 8.094 1.00 0.00 H MOTA 5433 2HG1 ILE B 170 -20.748 53.323 1.00 7.909 0.00 H ATOM 5434 1HG2 ILE B 170 -23.219 52.342 10.855 1.00 0.00 Н ATOM 5435 2HG2 ILE B 170 -22.796 53.819 11.714 1.00 0.00 H 40 ATOM 5436 3HG2 ILE B 170 -23.675 53.912 10.210 1.00 0.00 H 5437 1HD1 ILE B 170 MOTA -23.115 54.369 7.070 1.00 0.00 H 5438 2HD1 ILE B 170 ATOM -23.131 55.124 1.00 8.651 0.00 H ATOM 5439 3HD1 ILE B 170 -21.776 55.394 7.510 1.00 0.00 H ATOM LYS B 171 5440 N -22.156 55.999 11.475 1.00 0.52 N 45 ATOM 5441 CA LYS B 171 -22.902 57.220 11.537 1.00 0.52 C MOTA 5442 С LYS B 171 -21.908 58.330 11.406 1.00 0.52 С ATOM 5443 0 58.418 LYS B 171 -20.957 12.180 1.00 0.52 0 ATOM 5444 CB LYS B 171 -23.649 57.356 12.879 1.00 0.52 C ATOM 5445 CG LYS B 171 -24.731 58.436 12.935 1.00 0.52 C 50 ATOM 5446 CD LYS B 171 -24.206 59.860 12.790 1.00 0.52 C MOTA 5447 CE LYS B 171 -25.263 60.932 13.064 1.00 0.52 ATOM -26.436 -22.064 5448 NZ LYS B 171 60.713 12.190 1.00 0.52 N1+ ATOM 5449 LYS B 171 H 55.447 12.309 1.00 0.00 H ATOM 5450 HA LYS B 171 -23.632 57.218 10.707 1.00 0.00 H 55 ATOM 5451 1HB LYS B 171 -22.872 57.525 13.643 1.00 0.00 H ATOM 5452 2HB LYS B 171 -24.129 56.387 13.070 1.00 0.00 H ATOM 5453 1HG LYS B 171 -25.345 58.368 13.836 1.00 0.00 H ATOM 5454 2HG LYS B 171 -25.440 58.243 12.108 1.00 0.00 Н MOTA 5455 1HD LYS B 171 -23.965 59.931 11.730 1.00 0.00 н 60 MOTA 5456 2HD LYS B 171 -23.301 60.050 13.389 1.00 0.00 H ATOM 5457 1HE LYS B 171 -24.878 61.943 12.854 1.00 0.00 H ATOM 5458 2HE LYS B 171 -25.630 60.929 14.101 1.00 0.00 H ATOM 5459 1HZ LYS B 171 -27.152 61.412 12.333 1.00 0.00 H ATOM 5460 2HZ LYS B 171 -26.17460.754 11.214 1.00 0.00 H 65 MOTA 5461 3HZ LYS B 171 -26.861 59.813 12.366 1.00 0.00 H ATOM 5462 N ALA B 172 -22.097 59.199 10.393 1.00 0.31 ATOM 5463 CA ALA B 172 -21.148 60.249 10.164 1.00 0.31 C ATOM ALA B 172 5464 C -21.773 61.594 10.514 1.00 0.31 C ATOM 5465 0 **ALA B 172** -21.349 62.615 9.889 1.00 0.31 0 70 ATOM 5466 CB ALA B 172 -20.692 60.342 8.698 1.00 0.31 C MOTA 5467 OXT ALA B 172

-22.672

61.637

11.410

1.00

0.31

01-

5	ATOM ATOM ATOM ATOM ATOM ATOM	5469 HA 5470 1HB 5471 2HB	ALA B 172 ALA B 172 ALA B 172 ALA B 172 ALA B 172	-20.253 -19.856 -20.320	60.101 61.055 59.375	10.785 8.602 8.320	1.00 1.00 1.00	0.00 0.00	н н н н
	TER						2100	0.00	•••

TABLE 5

REMARK Model of Fc Gamma Receptor type IIIb; V.C. Epa, Feb 02, 1999. REMARK r3b_mod8.B99990013.pdb 1 REMARK Produced by MODELLER: 02-Feb-99 01:55:11 REMARK MODELLER OBJECTIVE FUNCTION: 933.2556 5.582 1.00 0.75 7.009 1.00 0.75 78.544 15G 2 1 N ARG 1 36.333 CA ARG 1 36.665 78.748 13G 3 2 MOTA 1.00 0.75 1.SG MOTA 3 CB ARG 1 37.362 80.102 7.211 4 6.455 1.00 0.75 15G 5 38.684 80.236 ARG MOTA 4 CG 1 ARG 39.381 81.577 6.691 1.00 0.75 1SG 5 CD 1 5 ATOM 1.00 0.75 1.SG 7 NE ARG 38.454 82.648 6.231 MOTA 6 CZ ARG 83.911 1.00 0.75 1SG 8 38.575 6.733 ATOM 7 1 0.75 1.00 1SG 9 8 NH1 ARG 1 39.561 B4.195 7.632 MOTA 1.00 0.75 15G 10 9 NH2 ARG 1 37.706 84.888 6.342 MOTA 7.815 1.00 0.75 15G 11 10 ARG 1 35.413 78.755 MOTA C 78.125 7.448 1.00 0.75 1SG 12 11 Ó ARG 1 34.422 MOTA 8.957 1.00 0.84 1SG 13 THR 35.435 79.465 12 N 2 MOTA 9.758 1.00 0.84 15G CA THR 2 34.253 79.541 14 MOTA 13 15 CB THR 2 34.507 79.998 11.165 1.00 0.84 1.SG MOTA 14 0.84 35.036 81.316 11.165 1.00 1SG 16 OG1 THR 2 MOTA 15 35.505 79.029 11.821 1.00 0.84 15G 17 15 CG2 THR 2 MOTA 9.098 1.00 0.84 18G 18 33.378 80.548 MOTA 17 С THR 2 15G 19 THR 2 33.857 81.407 8.359 1.00 0.84 18 n ATOM 0.71 19 N GLU 3 32.057 80.458 9.329 1.00 15G 20 MOTA 1.00 1SG 0.71 21 8.699 20 CA GLU 3 31.181 B1.396 MOTA 3 29.830 80.782 8.299 1.00 0.71 1SG 22 GLU MOTA 21 CB 29.965 79.711 7.214 1.00 0.71 1SG 23 CG GLU 3 ATOM 22 5.972 1.00 0.71 15G 24 30.554 80.365 MOTA 23 CD GLU 3 0.71 1SG 25 30.739 81.612 5.991 1.00 24 OE1 GLU 3 ATOM 1.00 0.71 1.56 26 30.827 79.627 4.988 25 OEZ GLU 3 MOTA 9.675 1.00 0.71 1SG 27 26 C GLU 3 30.937 B2.497 MOTA 28 10.753 1.00 0.71 1SG 3 30.388 82.277 27 0 GLU ATOM 1SG 29 1,00 0.37 ASP 31.367 83.722 9.318 28 N 4 ATOM 0.37 15G 30 84.828 10.215 1.00 asp 31.218 CA 4 ATOM 29 30 CB ASP 4 31.857 86.122 9.684 1.00 0.37 1SG 31 MOTA 1.00 0.37 13G 32 85.958 9.723 ATOM 31 CG ASP 4 33.370 85.029 10.428 1.00 0.37 15G 33 33.845 OD1 ASP MOTA 32 4 1SG 9.055 1.00 0.37 34 33 ODZ ASP 4 34.070 85.765 MOTA 1.00 0.37 1SG 35 85.099 10.401 ASP 4 29.767 MOTA 34 C 0.37 1.5G 36 4 29.251 85.050 11.516 1.00 MOTA 35 0 ASP 156 0.17 37 5 29.059 85.370 9.294 1.00 36 N LEU MOTA 9.399 1.00 0.17 15G 38 27.667 85.668 MOTA 37 CA LEU 5 8.075 1.00 0.17 15G 39 38 CB LEU 5 27.075 86.177 MOTA 0.17 1SG 40 87.486 7.592 1.00 LEU 5 27.732 MOTA 39 CG 1.00 0.17 15G 41 5 27.709 88.560 8.693 CD3 LEU ATOM 40 27.115 87.974 6.271 1.00 0.17 1SG 42 41 CD1 LEU 5 MOTA 15G 1.00 0.17 43 26.999 84.375 9.734 MOTA 42 С LEU 5 9.290 1.00 0.17 1**5**G 44 5 27.436 83.315 43 ٥ LEU MOTA 1SG 45 0.32 10.491 1.00 MOTA 44 N PRO 6 25.939 84.428 83.214 10.886 1.00 0.32 15G 46 PRO 5 25.286 45 CA MOTA 47 46 CD PRO 6 25.749 85.492 11.462 1.00 0.32 1SG ATOM 1SG 48 0.32 1.00 PRO б 24.243 83.628 11.919 ATOM 47 CB 0.32 15G 49 24.865 84.882 12.566 1.00 PRO 6 MOTA 48 CG 50 9.679 1.00 0.32 15G 49 PRO 5 24.755 82.520 MOTA Ċ 8.672 1.00 0.32 1\$G 51 24.506 83.182 MOTA 50 О PRO б 1.00 24.503 0.49 1SG 52 81.184 9.741 LYS 7 MOTA 51 N 1.00 0.49 1.SG 53 7 24.184 80.476 8.572 52 CA LYS MOTA 0.49 24.543 78.979 8.570 1.00 1\$Ġ 54 53 CB LYS 7 MOTA 0.49 1SG 55 78.697 8.611 1.00 7 26.045 54 CG LYS MOTA 0.49 15G 56 8.617 1.00 LYS 7 26.398 77.211 55 CD MOTA 25.652 76.398 0.49 15G 57 9.573 1.00 7 LYS MOTA 56 CE 0.49 LYS 26.238 76.623 11.012 1.00 1SG 58 57 NZ MOTA

ATOM	58	С	LYS	7	22.703	80.560	8.420	1.00	0.49		1 S G	59
ATOM	59	0	LYS	7	21.958	80.622	9.397	1.00	0.49		15G	60
ATOM	60	N	ALA	8	22.243	80.568	7.155	1.00	0.29		1SG	61
	61	CA	ALA	å	20.838	80.543	6.890	1.00	0.29		15G	62
ATOM											_	
ATOM	62	CB	ALA	8	20.483	80.789	5.413	1.00	0.29		1SG	63
ATOM	63	C	ALA	8	20.394	79.162	7.254	1.00	0.29		1SG	64
ATOM	64	0	ALA	8	21.215	78.248	7.328	1.00	0.29		15G	65
ATOM	65	N	VAL	9	19.086	78.978	7.532	1.00	0.10		15G	56
ATOM	66	CA	VAL	9	18.614	77.679	7.929	1.00	0.10		1 S G	67
ATOM	67	CB	VAL	9	18.031	77.676	9.312	1.00	0.10		150	68
	68		VAL	9	17.521	76.263	9.638	1.00	0.10		13G	69
MOTA												
MOTA	69	CGZ		9	19.104	78.190	10.287	1.00	0.10		150	70
atom	70	C	VAL	9	17.537	77.242	6.979	1.00	0.10		1SG	71
ATOM	71	0	VAL	9	16.568	77.964	5.746	1.00	0.10		15G	72
ATOM	72	N	VAL	10	17.674	76.015	6.431	1.00	0.19		15G	73
ATOM	73	CA	VAL	10	15.740	75.508	5.463	1.00	0.19		15G	74
ATOM	74	CB	VAL	10	17.398	74.689	4.392	1.00	0.19		1SG	75
ATOM	75		VAL	10	16.311	74.126	3.461	1.00	0.19		15G	76
ATOM	76		VAL	10	18.435	75.572	3.678	1.00	0.19		1SG	77
ATOM	77	С	VAL	10	15.729	74.538	6.147	1.00	0.19		1SG	78
ATOM	78	0	VAL	10	16.071	73.734	6.909	1.00	0.19		1SG	79
ATOM	79	N	PHE	11	14.436	74.903	5.866	1.00	0.29		1 S G	80
ATOM	80	CA	PHE	11	13.341	74.203	6.478	1.00	0.29		156	81
ATOM	81	CB	PHE	11	12.390	75.198	7.171	1.00	0.29		1SG	82
ATOM	82	CG	PHE	11	11.324	74.489	7.929	1.00	0.29		15G	83
	83		PHE	11	11.626	73.789	9.074	1.00	0.29		1SG	84
ATOM									0.29		1SG	85
ATOM	84		PHE	11	10.016	74.560	7.515	1.00				
MOTA	85		PHE	11	10.640	73.144	9.783	1.00	0.29		15G	86
MOTA	86		PHE	11	9.030	73.918	8.223	1.00	0.29		1SG	87
ATOM	87	cz	PHE	11	9.337	73.205	9.357	1.00	0.29		1SG	88
ATOM	88	Ċ	PHE	11	12.610	73.473	5.386	1.00	0.29		1 <i>5</i> G	89
ATOM	89	0	PHE	11	12.366	74.029	4.317	1.00	0.29		15G	90
ATOM	90	N	LEU	12	12.252	72.194	5.639	1.00	0.22		1SG	91
ATOM	91	CA	LEU	12	11.623	71.357	4.649	1.00	0.22		1SG	92
	92	CB	LEU	12	12.417	70.050	4.443	1.00	0.22		15G	93
ATOM									0.22		15G	94
ATOM	93	CG	LEU	12	11.841	69.069	3.405	1.00				
MOTA	94	CDZ		12	12.543	67.702	3.485	1.00	0.22		1 <i>5</i> G	95
ATOM	95	CD1	LEU	12	11.878	69.665	1.988	1.00	0.22		15G	96
ATOM	96	C	LEU	12	10.245	70.996	5.122	1.00	0.22	:	1SG	97
ATOM	97	0	LEU	12	10.069	70.535	6.248	1.00	0.22	:	15G	98
ATOM	98	N	GLU	13	9.214	71.217	4.272	1.00	0.16	:	1.SG	99
ATOM	99	CA	GLU	13	7.873	70.835	4.636	1.00	0.16	•	1SG	100
ATOM	100	CB	GLU	13	6.922	72.012	4.907	1.00	0.16		1.SG	
			GLU	13	7.239		6.177	1.00	0.16		15G	
ATOM	101	CG				72.794					LSG	
ATOM	102	CD	GLU	13	5.214	73.912	6.297	1.00	0.16			
ATOM	103		GLU	13	4.999	73.592	6.393	1.00	0.16			104
ATOM	104	OE2		13	6.630	75.102	6.291	1.00	0.15		1 S G	
atom	105	C	GLU	13	7.271	70.102	3.478	1.00	0.16		1SG	
ATOM	105	Q	GLU	13	7.330	70.573	2.342	1.00	0.15		15G	
MOTA	107	N	PRO	14	6.706	68.948	3.714	1.00	0.21		15G	108
MOTA	108	CA	PRO	14	6.667	68.302	4.995	1.00	0.21		1SG	109
ATOM	109	CD	PRO	14	5.925	68.248	2.709	1.00	0.21		1SG	110
ATOM	110	CB	PRO	14	5.700	67.126	4.839	1.00	0.21		LSG	
MOTA	111	CG	PRO	14	5.667	66.862	3.323	1.00	0.21		LSG	
					8.071				0.21		LSG	
MOTA	112	C	PRO	14		67.870	5.287	1.00				
ATOM	113	0	PRO	14	8.917	67.954	4.402	1.00	0.21		LSG	
ATOM	114	N	GLN	15	8.326	67.394	5.518	1.00	0.25		LSG	
MOTA	115	CA	GLN	15	9.620	67.052	7.049	1.00	0.25		1.SG	
ATOM	116	CB	GLN	15	9.550	66.690	8.541	1.00	0.25		LSG	
ATOM	117	CG	GLN	15	9.071	67.839	9.430	1.00	0.25	J	LSG	118
ATOM	118	CD	GLN	15	9.049	67.340	10.867	1.00	0.25	3	LSG	119

ATOM	119	OE1	GLN	15	9.139	68.123	11.812	1.00	0.25	1SG 120
ATOM	120	NE2	GLN	15	8.927	65.996	11.040	1.00	0.25	1SG 121
ATOM	121	C	GLN	15	10.263	65.875		1.00	0.25	15G 122
ATOM	122	0	GLN	15	11.479	65.714		1.00	0.25	1SG 123
ATOM	123	N	TRP	16	9.473	64.991		1.00	0.44	1SG 124
ATOM	124	CA	TRP	16	9.960	63.744		1.00	0.44	13G 125
	125	CB	TRP	16	8.870	63.744				
ATOM								1.00	0.44	15G 126
ATOM	126	CG	TRP	16	7.568	62.935		1.00	0.44	1SG 127
ATOM	127	CD2		16	7.393	62.263		1.00	0.44	15G 128
ATOM	128		TRP	16	6.368	63.510		1.00	0.44	1SG 129
ATOM	129		TRP	16	5.454	63.236		1.00	0.44	1SG 130
ATOM	130	CE2		16	6.072	62.471		1.00	0.44	1SG 131
ATOM	131		TRP	16	8.263	61.541		1.00	0.44	1SG 132
ATOM	132	CZZ		16	5.599	61.956		1.00	0.44	15G 133
ATOM	133	CZ3		16	7.780	61.015	8.351	1.00	0.44	1SG 134
ATOM	134	CHZ	TRP	16	6.473	61.220	8.745	1.00	0.44	1SG 135
MOTA	135	C	TRP	16	11.131	63.929	4.267	1.00	0.44	1SG 136
ATOM	136	0	TRP	16	11.062	64.584	3.297	1.00	0.44	1SG 137
ATOM	137	N	TYR	17	12.261	63.242	4.567	1.00	0.57	1SG 138
ATOM	138	CA	TYR	17	13.440	63.252	3.737	1.00	0.57	1SG 139
MOTA	139	CB	TYR	17	14.749	62.870		1.00	0.57	15G 140
ATOM	140	CG	TYR	17	14.639	61.516	5.071	1.00	0.57	1SG 141
ATOM	141		TYR	17	14.599	60.383	4.291	1.00	0.57	15G 142
MOTA	142	CDZ	TYR	17	14.615	61.383	5.440	1.00	0.57	1SG 143
ATOM	143	CEI	TYR	17	14.507	59.139	4.869	1.00	0.57	15G 144
ATOM	144	CEZ	TYR	17	14.524	60.142	7.024	1.00	0.57	15G 145
ATOM	145	CZ	TYR	17	14.455	59.017	6.237	1.00	0.57	15G 146
ATOM	146	OH	TYR	17	14.370	57.742	6.833	1.00	0.57	15G 147
ATOM	147	C	TYR	17	13.280	62.371	2.530	1.00	0.57	15G 148
		0	TYR	17	13.200					
MOTA	148					62.621	1.498	1.00	0.57	15G 149
ATOM	149	N	SER	18	12.494	61.278	2.632	1.00	0.33	1SG 150
ATOM	150	CA	SER	18	12.317	60.414	1.493	1.00	0.33	1SG 151
MOTA	151	CB	SER	18	12.454	58.918	1.826	1.00	0.33	1 SG 152
ATOM	152	OG-	SER	18	11.412	58.518	2.704	1.00	0.33	1SG 153
ATOM	153	C	SER	18	10.925	60.641	0.986	1.00	0.33	15G 154
MOTA	154	0	SER	18	9.960	60.479	1.730	1.00	0.33	18G 155
ATOM	155	N	VAL	19	10.783	61.019	-0.304	1.00	0.11	1SG 156
ATOM	156	CA	VAL	19	9.477	61.311	-0.838	1.00	0.11	1SG 157
ATOM	157	CB	VAL	19	9.269	62.761	-1.167	1.00	0.11	15G 158
ATOM	158	CG1	VAL	19	9.380	63.581	0.130	1.00	0.11	1SG 159
ATOM	159	CG2	VAL	19	10.274	53.169	-2.257	1.00	0.11	1SG 160
ATOM	160	C	VAL	19	9.271	60.547	-2.114	1.00	0.11	1SG 151
ATOM	161	0	VAL	19	10.165	59.855	-2.599	1.00	0.11	1SG 162
ATOM	162	N	LEU	20	8.048	60.648	-2.680	1.00	0.12	18G 163
ATOM	163	CA	LEU	20	7.707	59.953	-3.890	1.00	0.12	15G 164
ATOM	154	CB	LEU	20	6.371	59.199	-3.799	1.00	0.12	1SG 165
ATOM	165	CG	LEU	20	6.393	58.029	-2.795	1.00	0.12	1SG 166
ATOM	166	CD2		20	7.551	57.064	-3.096	1.00	0.12	15G 167
ATOM	167	CD1		20	5.036	57.311	-2.743	1.00	0.12	1SG 168
ATOM	168	C	LEU	20	7.584	60.945	-5.006	1.00	0.12	15G 169
ATOM	169	ō	LEU	20	7.318	62.129	-4.797	1.00	0.12	1SG 170
ATOM	170	N	GLU	21	7.793	60.471	-6.250	1.00	0.27	1SG 171
ATOM	171	CA	GLU	21	7.682	61.341	-7.379	1.00	0.27	18G 172
ATOM	172	CB	GLU	21	7.865	60.617	-8.725	1.00	0.27	1SG 173
ATOM	173	CG	GLU	21	9.271	60.049	-8.935	1.00	0.27	15G 173
ATOM	174		GLU	21	9.297		-10.297	1.00	0.27	1SG 175
ATOM	175	OE1		21	8.246	59.409		1.00	0.27	1SG 176
	176	OEZ		21	10.363		-10.550		0.27	1SG 176 1SG 177
ATOM								1.00		
ATOM	177		GLU	21	6.305	61.919	-7.359	1.00	0.27	15G 178
ATOM	178	0	GLU	21	5.336	61.251	-7.002	1.00	0.27	19G 179
MOTA	179	N	LYS	22	6.206	63.202	-7.752	1.00	0.41	1SG 180

ATOM	180	CA	LYS	22	4.977	53.941	-7.839	1.00	0.41	1SG 181
ATOM	181	CB	LYS	22	3.802	63.104	-8.379	1.00	0.41	1SG 182
ATOM	182	CG	LYS	22	2.521	63.919	-8.568	1.00	0.41	15G 183
ATOM	183	CD	LYS	22	1.471	63.227	-9.442	1.00	0.41	1SG 184
ATOM	184	CE	LYS	22	1.782	63.301	-10.939	1.00	0.41	1SG 185
ATOM	185	NZ	LYS	22	0.726	62.510	-11.713	1.00	0.41	1SG 186
ATOM	186	C	LYS	22	4.576	64.522	-6.511	1.00	0.41	1SG 187
ATOM	187	ō	LYS	22	3.617	65.290	-6.454	1.00	0.41	1SG 188
ATOM	188	N	ASP	23	5.298	64.220	-5.413	1.00	0.26	1SG 189
ATOM	189	CA	ASP	23	4.948	64.822	-4.152	1.00	0.26	1SG 190
ATOM	190	CB	ASP	23	5.586	64.148	-2.931	1.00	0.26	15G 191
	191	CG	ASP	23	4.923	62.800	-2.666	1.00	0.26	1SG 192
ATOM	192		ASP	23	3.763	62.602	-3.117	1.00	0.26	1SG 193
ATOM			ASP	23	5.574	51.949	-2.004	1.00	0.26	19G 194
ATOM	193			23	5.437	66.242	-4.163	1.00	0.26	1SG 195
MOTA	194	C	ASP	23	6.388	66.584	-4.872	1.00	0.25	1SG 196
ATOM	195	0	ASP			67.104	-3.350	1.00	0.11	15G 197
ATOM	196	N	SER	24	4.784			1.00	0.11	19G 198
atom	197	CA	SER	24	5.124	68.497	-3.284		0.11	15G 199
MOTA	198	CB	SER	24	3.932	69.399	-2.918	1.00		15G 200
atom	199	OG	SER	24	4.336	70.760	-2.873	1.00	0.11	
ATOM	200	С	SER	24	6.159	68.680	-2.222	1.00	0.11	15G 201
ATOM	201	0	5ER	24	6.104	68.045	-1.171	1.00	0.11	1SG 202
ATOM	202	N	VAL	25	7.164	69.537	-2.487	1.00	0.10	1SG 203
ATOM	203	CA	VAL	25	8.167	69.792	-1.492	1.00	0.10	1SG 204
ATOM	204	CB	VAL	25	9.530	69.287	-1.877	1.00	0.10	1SG 205
ATOM	205	CG1	VAL	25	10.534	69.704	-0.789	1.00	0.10	1SG 206
ATOM	206	CG2	VAL	25	9.453	67. 76 7	-2.104	1.00	0.10	18G 207
ATOM	207	C	VAL	25	8.278	71.276	-1.344	1.00	0.10	1SG 208
ATOM	208	0	VAL	25	8.336	71.999	-2.338	1.00	0.10	15G 209
ATOM	209	N	THR	26	8.295	71.766	-0.084	1.00	0.09	1SG 210
ATOM	210	CA	THR	26	8.408	73.177	0.164	1.00	0.09	15G 211
ATOM	211	CB	THR	26	7.254	73.732	0.945	1.00	0.09	15G 212
ATOM	212	QG1	THR	26	6.040	73.502	0.247	1.00	0.09	1SG 213
MOTA	213	CG2	THR	26	7.467	75.243	1.142	1.00	0.09	18G 214
ATOM	214	C	THR	26	9.640	73.398	0.982	1.00	0.09	15G 215
ATOM	215	0	THR	26	9.791	72.851	2.073	1.00	0.09	1SG 216
ATOM	216	N	LEU	27	10.568	74.219	0.461	1.00	0.16	1SG 217
ATOM	217	CA	LEU	27	11.777	74.529	1.162	1.00	0.16	15G 218
ATOM	218	CB	LEU	27	13.031	74.380	0.286	1.00	0.16	1SG 219
ATOM	219	CG	LEU	27	13.325	72.930	-0.140	1.00	0.16	15G 220
ATOM	220	CD2	LEU	27	13.423	72.00B	1.081	1.00	0.16	15G 221
ATOM	221		LEU	27	14.585	72.854	-1.013	1.00	0.16	15G 222
MOTA	222	C	LEU	27	11.583	75.974	1.550	1.00	0.16	1SG 223
ATOM	223	0	LEU	27	11.267	76.812	0.752	1.00	0.16	15G 224
ATOM	224	N	LYS	28	12.051	76.300	2.806	1.00	0.26	15G 225
ATOM	225	CA	LYS	28	11.982	77.664	3.253	1.00	0.26	15G 226
ATOM	226	CB	LYS	28	11.025	77.848	4.443	1.00	0.26	1SG 227
ATOM	227	CG	LYS	2 B	9.559	77.562	4.112	1.00	0.26	15G 228
ATOM	228	CD	LYS	28	8.696	77.332	5.355	1.00	0.26	1SG 229
ATOM	229	CE	LYS	28	8.759	78.477	6.369	1.00	0.26	15G 230
ATOM	230	NZ	LYS	28	7.898	78.171	7.534	1.00	0.26	1SG 231
ATOM	231	C	LYS	28	13.350	78.065	3.716	1.00	0.26	1SG 232
	232	ŏ	LYS	28	13.972	77.361	4.510	1.00	0.26	15G 233
ATOM ATOM	233	N	CYS	29	13.855	79.221	3.231	1.00	0.25	15G 234
	234	CA	CYS	29	15.166	79.665	3.623	1.00	0.25	1SG 235
ATOM	235	CB	CYS	29	15.989	80.261	2.466	1.00	0.25	1SG 236
ATOM	235	SG	CYS	29	17.746	80.487	2.876	1.00	0.25	1SG 237
atom atom	237	C	CY5	29	14.976	80.743	4.635	1.00	0.25	1SG 238
		0	CYS	29	14.520	81.842	4.318	1.00	0.25	1SG 239
MOTA	238		GLN	30	15.362	80.444	5.888	1.00	0.20	1SG 240
ATOM	239 240	N CA	GLN	30	15.150	81.352	6.974	1.00	0.20	1SG 241
ATOM	240	CA.	GUIN	50	20.200	·				

						233					
MOTA	241	CB	GLN	30	14.652	80.641	8.250	1.00	0.20	15G 24	
ATOM	242	CG	GLN	30	13.328	79.910	8.073	1.00	0.20	15G 24 15G 24	
ATOM	243	CD	GLN GLN	30 30	12.990 13.436	79.231 79.665	9.393 10.454	1.00	0.20	15G 24	
ATOM ATOM	244 245	NE2		30	12.190	78.133	9.331	1.00	0.20	1SG 24	
ATOM	246	C	GLN	30	16.447	82.021	7.307	1.00	0.20	15G 24	7
ATOM	247	0	GLN	30	17.516	81.416	7.227	1.00	0.20	18G 24	
ATOM	248	N	GLY	31	16.370	83.318	7.670	1.00	0.17	15G 24	
MOTA	249	CA	GLY	31	17.534	84.063	8.057	1.00	0.17	15G 25 15G 25	
ATOM	250	C	GLY	31	17.314 16.372	85.486 85.790	7.647 6.917	1.00	0.17	15G 25	
ATOM ATOM	251 252	Ŋ	GLY ALA	31 32	18.204	86.394	8.100	1.00	0.26	1SG 25	
ATOM	253	CA	ALA	32	18.069	87.786	7.779	1.00	0.26	1SG 25	
ATOM	254	CB	ALA	32	19.036	88.698	8.555	1.00	0.26	15G 25	
ATOM	255	C	ALA	32	18.361	87.941	6.323	1.00	0.26	18G 25	
ATOM	256	0	ALA	32	19.239 17.622	87,270 88.851	5.783 5.656	1.00	0.25 0.37	1SG 25 1SG 25	
ATOM	257 258	N CA	TYR TYR	33 33	17.742	89.029	4.237	1.00	0.37	1sg 25	
atom atom	259	CB	TYR	33	16.403	88.888	3.494	1.00	0.37	1SG 26	
MOTA	260	CG	TYR	33	15.701	87.652	3.939	1.00	0.37	1SG 26	
ATOM	261	CD1		33	16.014	86.413	3.431	1.00	0.37	15G 26	
MOTA	262	CD2	TYR	33	14.701	87.754	4.878	1.00	0.37	1SG 26 1SG 26	
ATOM	263	CEL	TYR	33	15.336	85.295 86.542	3.863 5.313	1.00	0.37 0.37	1SG 26	
MOTA	264	CE2	TYR TYR	33 33	14.020 14.340	85.408	4.804	1.00	0.37	15G 26	
atom atom	265 266	OH	TYR	33	13.646	84.261	5.243	1.00	0.37	15G 26	
ATOM	267	C	TYR	33	18.105	90.462	3.998	1.00	0.37	1SG 26	
MOTA	258	0	TYR	33	18.011	91.297	4.896	1.00	0.37	15G 26	
MOTA	269	N	SER	34	18.565	90.773	2.768	1.00	0.30	15G 27 15G 27	
MOTA	270	CA	SER	34	18.837 19.977	92.136 92.293	2.411 1.390	1.00	0.30	15G 27	
ATOM ATOM	271 272	CB OG	SER SER	34 34	21.202	91.842	1.949	1.00	0.30	15G 27	
ATOM	273	Ç	SER	34	17.592	92.564	1.776	1.00	0.30	1SG 27	
ATOM	274	ō	SER	34	16.777	91.896	1.264	1.00	0.30	1SG 27	
ATOM	275	N	PRO	35	17.383	93.950	1.821	1.00	0.24	18G 27	
MOTA	276	CA	PRO	35	16.224	94.476	1.167	1.00	0.24	1SG 27 1SG 27	
ATOM	277	CD	PRO	35	17.816	94.788 95.891	2.923 1.717	1.00	0.24	15G 27	9
MOTA	278 279	CB CG	PRO PRO	35 35	16.024 17.306	96.182	2.527	1.00	0.24	1SG 28	
MOTA MOTA	280	C	PRO	35	16.414	94.377	-0.309	1.00	0.24	18G 28	
ATOM	281	ō	PRO	35	17.086	95.235	-0.882	1.00	0.24	1SG 28	
ATOM	282	N	GLU	36	15.796	93.358	-0.938	1.00	0.28	1SG 28 1SG 28	
ATOM	283	CA	GLU	36	15.884	93.180	-2.356	1.00	0.28 0.28	1SG 28	_
ATOM	284 285	CB CG	GLU GLU	36 36	17.245 17.579	92.670 91.245	-2.865 -2.422	1.00	0.28	1SG 28	
atom atom	286	CD	GLU	36	18.911	90.662	-3.049	1.00	0.28	15G 28	
ATOM	287		GLU	36	18.954	90.706	-4.299	1.00	0.28	1SG 28	
MOTA	288	OE2	GLU	36	19.906	90.723	-2.288	1.00	0.28	15G 28	
ATOM	389	C	GLU	36	14.878	92.137	-2.725	1.00	0.28	1SG 29 1SG 29	
ATOM	290	0	GLU	36	14.517	91.286	-1.912 -3.978	1.00	0.28	15G 29	
ATOM	291 292	N CA	asp asp	3 7 37	14.393 13.415	92.191 91.251	-4.436	1.00	0.30	1SG 29	
MOTA MOTA	292	CB	ASP	37	12.885	91.582	-5.842	1.00	0.30	15G 29	4
ATOM	294	CG	ASP	37	11.706	90.567	-6.145	1.00	0.30	15G 29	
ATOM	295	OD1	ASP	37	11.405	89.773	-5.310	1.00	0.30	15G 29	
MOTA	296		ASP	37	11.086	90.853	-7.226	1.00	0.30	15G 29 15G 29	
ATOM	297	C	asp asp	37 37	14.020 13.423	89.882 88.916	-4.499 -4.026	1.00	0.30	15G 29	
ATOM ATOM	298 299	N O	ASN	37 38	15.227	89.754	-5.088	1.00	0.32	1SG 30	
ATOM	300	CA	ASN	38	15.808	88.444	-5.198	1.00	0.32	1SG 30	1
ATOM	301	СВ	ASN	38	16.651	88.257	-6.472	1.00	0.32	1SG 30	2

MOTA	302	CG	ASN	38	15.715	88.249	-7.675	1.00	0.32	1SG 303
ATOM	303	OD1	ASN	38	14.501	88.106	-7.540	1.00	0.32	1SG 304
ATOM	304		ASN	38	16.300	88.393	-8.894	1.00	0.32	15G 305
ATOM	305	С	ASN	38	16.722	88.253	-4.028	1.00	0.32	15G 306
ATOM	306	ō	ASN	38	17.941	88.343	-4,157	1.00	0.32	1SG 307
ATOM	307	N	SER	39	16.129	87.978	-2.851	1.00	0.48	1SG 308
ATOM	308	CA	SER	39	16.810	87.823	-1.597	1.00	0.48	15G 309
	309	CB	SER	39	15.861	87.925	-0.392	1.00	0.48	1SG 310
ATOM				39	15.314	89.231	-0.308	1.00	0.48	1SG 311
MOTA	310	og C	SER			86.510	-1.448	1.00	0.48	15G 312
ATOM	311	C	SER	39	17.535					1SG 312
ATOM	312	0	SER	39	18.534	86.442	-0.737	1.00	0.48	1SG 314
ATOM	313	N	THR	40	17.061	85.405	-2.055	1.00	0.54	
ATOM	314	CA	THR	40	17.721	84.170	-1.709	1.00	0.54	1SG 315
MOTA	315	CB	THR	40	16.821	83.202	-0.997	1.00	0.54	15G 316
ATOM	316	OGI	THR	40	15.745	82.821	-1.841	1.00	0.54	1SG 317
ATOM	317	.CG2	THR	40	16.283	83.878	0.276	1.00	0.54	1SG 318
ATOM	318	С	THR	40	18.276	83.447	-2.899	1.00	0.54	19G 319
atom	319	O	THR	40	17.733	83.482	-4.001	1.00	0.54	15G 320
MOTA	320	N	GLN	41	19.415	82.757	-2.678	1.00	0.31	15G 321
ATOM	321	CA	GLN	41	20.021	81.948	-3.694	1.00	0.31	15G 322
MOTA	322	CB	GLN	41	21.552	82.067	-3.738	1.00	0.31	1SG 323
MOTA	323	CG	GLN	41	22.071	83.453	-4.118	1.00	0.31	1SG 324
ATOM	324	CD	GLN	41	23.581	83.418	-3.944	1.00	0.31	1SG 325
ATOM	325	OEl	GLN	41	24.283	84.384	-4.235	1.00	0.31	1SG 326
ATOM	326	NE2	GLN	41	24.101	82.256	-3.443	1.00	0.31	1SG 327
ATOM	327	C	GLN	41	19.738	80.532	-3.297	1.00	0.31	15G 328
ATOM	328	ō	GLN	41	19.972	80.153	-2.150	1.00	0.31	15G 329
ATOM	329	N	TRP	42	19.207	79.715	-4.229	1.00	0.13	1SG 330
ATOM	330	CA	TRP	42	18.948	78.336	-3.910	1.00	0.13	15G 331
ATOM	331	СВ	TRP	42	17.531	77.840	-4.248	1.00	0.13	1SG 332
ATOM	332	CG	TRP	42	16.469	78.313	-3.291	1.00	0.13	1SG 333
MOTA	333	CDZ	TRP	42	16.139	77.634	-2.069	1.00	0.13	1SG 334
	334	CD1	TRP	42	15.660	79.406	-3.359	1.00	0.13	1SG 335
MOTA			TRP	42	14.849	79.450	-2.253	1.00	0.13	1SG 336
ATOM	335	NE1			15.130	78.368	-1.451	1.00	0.13	1SG 337
ATOM	336	CE2	TRP	42 42	16.638	76.495	-1.506	1.00	0.13	1SG 338
ATOM	337	CE3	TRP					1.00	0.13	15G 339
ATOM	338	CZZ		42	14.601	77.977	-0.255	1.00	0.13	15G 340
MOTA	339	CZ3	TRP	42	16.101	76.100	-0.301		0.13	15G 341
ATOM	340	CHZ	TRP	42	15.101	76.827	0.312	1.00		15G 341
ATOM	341	·Č	TRP	42	19.895	77.498	-4.701	1.00	0.13	15G 342
atom	342	0	TRP	42	20.228	77.832	-5.836	1.00	0.13	15G 343
ATOM	343	N	PHE	43	20.367	76.385	-4.099	1.00	0.11	
ATOM	344	CA	PHE	43	21.302	75.544	-4.787	1.00	0.11	1SG 345
ATOM	345	CB	PHE	43	22.711	75.557	-4.166	1.00	0.11	1SG 346
ATOM	346	CG	PHE	43	23.295	76.925	-4.278	1.00	0.11	15G 347
ATOM	347	CD1		43	23.030	77.879	-3.322	1.00	0.11	15G 348
ATOM	348	CD2	PHE	43	24.113	77.251	-5.335	1.00	0.11	1SG 349
ATOM	349	CE1		43	23.572	79.139	-3.421	1.00	0.11	15G 350
MOTA	350	CE3	PHE	43	24.658	78.510	-5.440	1.00	0.11	1SG 351
ATOM	351	cz	PHE	43	24.386	79.457	-4.482	1.00	0.11	15G 352
MOTA	352	C	PHE	43	20.843	74.120	-4.693	1,00	0.11	15G 353
ATOM	353	0	PHE	43	20.285	73.695	-3.682	1.00	0.11	15G 354
ATOM	354	N	HIS	44	21.065	73.353	- 5.782	1.00	0.13	1SG 355
ATOM	355	CA	HIS	44	20.777	71.948	-5.815	1.00	0.13	19G 356
ATOM	356	NDl	HIS	44	18.580	69.494	-7.813	1.00	0.13	15G 357
ATOM	357	CG	HIS	44	19.360	70.111	-6.859	1.00	0.13	1\$G 358
MOTA	358	CB	HIS	44	19.757	71.560	-6.902	1.00	0.13	1SG 359
ATOM	359	NE2		44	19.059	67.948	-6.288	1.00	0.13	1SG 360
ATOM	360	CD2	HIS	44	19.643	69.152	-5.935	1.00	0.13	15G 361
ATOM	361	CEI		44	18.432	68.203	-7.422	1.00	0.13	1SG 362
ATOM	362	C	HIS	44	22.070	71.286	-6.166	1.00	0.13	1SG 363

ATOM	363	0	HIS	44	22.582	71.465	-7.270	1.00	0.13	1SG 364
ATOM	364	N	ASN	45	22.633	70.494	-5.234	1.00	0.21	1SG 365
ATOM	365	CA	ASN	45	23.888	69.850	-5.489	1.00	0.21	1SG 366
ATOM	366	CB	ASN	45	23.811	68.784	-6.595	1.00	0.21	1SG 367
ATOM	367	CG	ASN	45	23.006	67.606	-6.063	1.00	0.21	1SG 368
ATOM	368		ASN	45	22.804	67.465	-4.857	1.00	0.21	1SG 369
ATOM	369	ND2		45	22.542	66.723	-6.987	1.00	0.21	1SG 370
ATOM	370	С	ASN	45	24.885	70.895	-5.896	1.00	0.21	1SG 371
ATOM	371	Ö	ASN	45	25.698	70.672	-6.792	1.00	0.21	1SG 372
ATOM	372	N	GLU	46	24.851	72.063	-5.223	1.00	0.25	15G 373
ATOM	373	CA	GLU	46	25.781	73.134	-5.465	1.00	0.25	15G 374
ATOM	374	CB	GLU	46	27.239	72.652	-5.580	1.00	0.25	15G 375
ATOM	375	CG	GLU	45	27.885	72.278	-4.245	1.00	0.25	1SG 376
ATOM	376	CD	GLU	46	28.429	73.558	-3.621	1.00	0.25	15G 377
ATOM	377	OE1	GLU	46	28.277	74.634	-4.260	1.00	0.25	1SG 378
ATOM	378	OE2	GLU	46	29.006	73.479	-2.503	1.00	0.25	1SG 379
ATOM	379	С	GLU	46	25.473	73.880	-6.731	1.00	0.25	15G 380
ATOM	380	0	GLU	46	26.222	74.785	-7.095	1.00	0.25	15G 381
ATOM	381	N	SER	47	24.354	73.575	-7.430	1.00	0.17	1SG 382
MOTA	382	CA	SER	47	24.095	74.317	-8.633	1.00	0.17	15G 383
ATOM	383	CB	SER	47	23.621	73.440	-9.805	1.00	0.17	15G 384
ATOM	384	QG	SER	47	24.655	72.553	-10.206	1.00	0.17	1SG 385
MOTA	385	C	SER	47	22.995	75.284	-8.328	1.00	0.17	1SG 386
MOTA	386	0	SER	47	21.985	74.922	-7.728	1.00	0.17	15G 387
ATOM	387	N	LEU	48	23.167	76.556	-8.743	1.00	0.23	15G 388
ATOM	388	CA	LEU	48	22.186	77.559	-8.441	1.00	0.23	18G 389
ATOM	389	CB	LEU	48	22.626	78.993	-8.790	1.00	0.23	19G 390
ATOM	390	CG	LEU	48	21.562	80.060	-8.465	1.00	0.23	1SG 391
ATOM	391	CD2	LEU	48	21.917	81.419	-9.089	1.00	0.23	15G 392
MOTA	392	CD1	LEU	48	21.311	80.151	-6.951	1.00	0.23	1SG 393
ATOM	393	C	LEU	48	20.947	77.283	-9.227	1.00	0.23	1SG 394
ATOM	394	0	LEU	48	21,009		-10.389	1,00	0.23	1SG 395
ATOM	395	N	ILE	49	19.775	77.464	-8.584	1.00	0.46	1SG 396
ATOM	396	CA	ILE	49	18.531	77.323	-9.283	1.00	0.46	15G 397
MOTA	397	CB	ILE	49	17.549	76.400	-8.612	1.00	0.46	1SG 398
ATOM	398	CG2	ILE	49	18.080	74.962	-8.702	1.00	0.46	1SG 399
ATOM	399	CG1	ILE	49	17.241	76.864	-7.186	1.00	0.46	1SG 400
atom	400	CD1		49	16.161	76.019	-6.512	1.00	0.46	1SG 401
ATOM	401	С	ILE	49	17.942	78.697	-9.391	1.00	0.46	1SG 402
ATOM	402	0	ILE	49	17.639	79.357	-8.403	1.00	0.45	15G 403
ATOM	403	N	SER	50	17.764		-10.636	1.00	0.56	15G 404
ATOM	404	CA	SER	50	17.325		-10.966	1.00	0.56	1SG 405
ATOM	405	CB	SER	50	17.505		-12.460	1.00	0.56	15G 406 15G 407
atom	406	OG	SER	50	18.882		-12.803	1.00	0.56	15G 408
ATOM	407	Ç	SER	50	15.878		-10.618	1.00	0.56 0.56	15G 409
ATOM	408	0	SER	50	15.446		-10.519	1.00		15G 410
ATOM	409	N	SER	51	15.082		-10.449 -10.325	1.00	0.61	15G 411
ATOM	410	CA	SER	51 51	13.649 13.004		-10.323	1.00	0.61	1SG 412
ATOM	411	CB	SER	51	13.266		-11.372	1.00	0.61	1SG 413
ATOM	412	OG	SER	51 51	13.097	80.566	-9.184	1,00	0.61	15G 414
ATOM	413	C	SER	51		81.348	-9.451	1.00	0.61	1SG 415
ATOM	414 61 5	0	ser Gln	51 52	12.185 13.569	80.481	-7.907	1.00	0.62	15G 416
ATOM	416	N CA	GLN	5∡ 52	12.750	81.193	-6.937	1.00	0.62	1SG 417
MOTA	417	CB	GLN	52 52	11.586	80.313	-6.439	1.00	0.62	15G 418
ATOM	418	CG	GLN	52 52	10.443	B1.071	-5.758	1.00	0.62	1SG 419
MOTA MOTA	419	CD	GLN	52	9.317	80.075	-5.510	1.00	0.62	1SG 420
ATOM	420		GLN	52	9.529	78.864	-5.547	1.00	0.62	1SG 421
ATOM	421	NE2	GLN	52	8.086	80.594	-5.258	1.00	0.62	15G 422
ATOM	422	C	GLN	52	13.480	81.759	-5.707	1.00	0.62	15G 423
ATOM	423	Ö	GLN	52	14.681	81.533	-5.549	1.00	0.62	15G 424
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ATOM	424	N	ALA	5 3	12.693	82.502	-4.835	1.00	0.57	15G 425
ATOM	425	CA	ALA	53	12.863	83.308	-3.621	1.00	0.57	1SG 426
ATOM	426	CB	ALA	5 3	11.846	84.457	-3.520	1.00	0.57	1SG 427
ATOM	427	c	ALA	53	12.782	82.536	-2.306	1.00	0.57	1SG 428
ATOM	428	0	ALA	53	13.156	81.373	-2.235	1.00	0.57	15G 429
ATOM	429	N	SER	54	12.284	83.191	-1.212	1.00	0.58	15G 430
ATOM	430	CA	SER	54	12.293	82.741	0.175	1.00	0.58	1SG 431
ATOM	431	CB	SER	54	11.521	83.693	1.105	1.00	0.58	1SG 432
ATOM	432	OG	SER	54	12.131	84.975	1.114	1.00	0.58	18G 433
ATOM	433	C	SER	54	11.680	81.388	0.356	1.00	0.58	1SG 434
ATOM	434	0	SER	54	12.214	80.553	1.090	1.00	0.58	15G 435
ATOM	435	N	SER	\$5	10.517	81.132	-0.255	1.00	0.46	1SG 436
ATOM	436	CA	SER	55	9.984	79.811	-0.133	1.00	0.46	1SG 437
ATOM	437	CB	SER	55	8.524	79.757	0.347	1.00	0.46	15G 438
ATOM	438	OG	SER	55	7.665	80.343	-0.518	1.00	0.46	18G 439
ATOM	439	C	SER	55	10.047	79.255	-1.508	1.00	0.46	15G 440
ATOM	440	0	SER	55	9.761	79.953	-2.479	1.00	0.46	15G 441
ATOM	441	N	TYR	56	10.485	77.992	-1.622	1.00	0.43	15G 442
ATOM	442	CA	TYR	56	10.595	77.372	-2.903	1.00	0.43	15G 443
ATOM	443	CB	TYR	56	12.067	77.058	-3.232	1.00	0.43	18G 444
ATOM	444	CG	TYR	56	12.177	76.276	-4.492	1.00	0.43	15G 445
ATOM	445		TYR	5 6	11.797	76.812	-5.701	1.00	0.43	15G 446
ATOM	445		TYR	56	12.710	75.010	-4.460	1.00	0.43	15G 447
ATOM	447	CEL	TYR	56	11.919	75.076	-6.857	1.00	0.43	1SG 448
ATOM	448	CE2	TYR	56	12.836	74.270	-5.612	1.00	0.43	1SG 449
ATOM	449	CZ	TYR	56	12.436	74.803	-6.814	1.00	0.43	18G 450
ATOM	450	OH	TYR	56	12.563	74.048	-8.000	1.00	0.43	15G 451
ATOM	451	С	TYR	5 6	9.801	76.113	-2.812	1.00	0.43	15G 452
ATOM	452	0	TYR	56	10.155	75.196	-2.074	1.00	0.43	15G 453
ATOM	453	N	PHE	57	8.684	76.046	-3.561	1.00	0.62	15G 454
ATOM	454	CA	PHE	57	7.847	74.888	-3.487	1.00	0.62	18G 455
ATOM	455	CB	PHE	57	6.421	75.206	-2.996	1.00	0.62	1SG 456
ATOM	455	CG	PHE	57	5.802	76.189	-3.932	1.00	0.62	15G 457
ATOM	457	CD1	PHE	57	5.086	75. 764	-5.028	1.00	0.62	15G 458
ATOM	458	CDZ	PHE	57	5.937	77.540	-3.710	1.00	0.62	1SG 459
ATOM	459	CE1	PHE	57	4.514	76.671	-5.889	1.00	0.62	1SG 460
MOTA	460	CE2	PHE	57	5.368	78.452	-4.567	1.00	0.62	1SG 461
ATOM	461	CZ	PHE	57	4.655	78.018	-5.659	1.00	0.62	15G 462 15G 463
MOTA	462	C	PHE	57	7.760	74.286	-4.644	1.00	0.62	15G 464
MOTA	463	O	PHE	57	7.588	74.986	-5.840	1.00	0.62	
ATOM	464	N	ILE	58	7.914	72.952	-4.921	1.00	0.54	1SG 465
MOTA	465	CA	ILE	58	7.8 07	72.349	-6,209	1.00	0.54	1SG 466
MOTA	456	CB	ILE	58	9.127	72.238	-6.929	1.00	0.54	1SG 467
ATOM	467	CG2	ILE	58	9.613	73.672	-7.192	1.00	0.54	1SG 468
MOTA	458	CG1	ILE	58	10.148	71.373	-6.163	1.00	0.54	15G 469
MOTA	469	CD1	ILE	58	9.908	69.865	-6.239	1.00	0.54	1SG 470
ATOM	470	¢	ILE	58	7.196	70.999	-6.075	1.00	0.54	1SG 471 1SG 472
ATOM	471	0	ILE	58	7.445	70.281	-5.109	1.00	0.54	1SG 473
ATOM	472	N	ASP	59	6.318	70.643	-7.038	1.00	0.34	15G 474
MOTA	473	CA	ASP	59	5.869	69.286	-7.121	1.00		1SG 475
ATOM	474	CB	ASP	59	4.410	69.150	-7.587	1.00	0.34	1SG 475
ATOM	475	CG	ASP	59	3.516	69.675	-6.473	1.00	0.34	15G 477
MOTA	476		ASP	59	4.061	70.282	-5.514	1.00	0.34	1SG 478
MOTA	477		ASP	59 50	2.277	69.465	-6.562	1.00	0.34	15G 479
atom	478	С	ASP	59	6.741	68.771	-8.189	1.00	0.34	1SG 480
ATOM	479	0	ASP	59	6.411	67.882	-8.972 -0.200	1.00	0.27	15G 481
ATOM	480	N	ALA	60	7.950	69.337	-8.208 -9.141	1.00	0.27	15G 482
ATOM	481	CA	ALA	60 60	8.903	68.892 69.945	-9.141 -9.459	1.00	0.27	18G 483
ATOM	482	CB	ALA	60 60	9.978 9 .569	67,769	-8.452	1.00	0.27	1SG 484
ATOM	483	C	ALA	60 60	10.713	57.472	-8.784	1.00	0.27	19G 485
ATOM	484	J	MUM	Q U		U ,	J U W	.		

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ATOM	485	N	ALA	61	8.892	67.133	-7.457	1.00	0.37	1SG 486
ATOM	486	CA	ALA	61	9.565	66.004	-6.941	1.00	0.37	1SG 487
ATOM	487	CB	ALA	61	8.825	65.293	-5.796	1.00	0.37	15G 488 15G 489
ATOM	488	C	ALA	61	9.623	65.065	-8.099	1.00	0.37	15G 490
ATOM	489	0	ALA	61	8.503	64.547	-8.550	1.00	0.56	1SG 491
ATOM	490	N	THR	62	10.842	64.876	-8.632 -9.750	1.00	0.56	1SG 492
MOTA	491	CA	THR	62	11.083	64.025 64.754		1.00	0.56	1SG 493
ATOM	492	CB	THR	62	11.287	65.617		1.00	0.56	15G 494
MOTA	493	OGI	THR	62	12.411	65.559	-11 364	1.00	0.56	1SG 495
ATOM	494	CG2	THR	62 62	10.016 12.357	63.334	-9.425	1.00	0.56	1SG 496
ATOM	495	C	THR THR	62	13.021	63.674	-8.449	1.00	0.56	1SG 497
ATOM	496	O N	VAL	63	12.743	62.358		1.00	0.52	1SG 498
MOTA	497 498	N CA	VAL	63	13.904	61.569	-9.983	1.00	0.52	15G 499
MOTA MOTA	499	CB	VAL	63	14.189	60.580	-11.080	1.00	0.52	150 500
ATOM	500		VAL	63	13.009	59.597	-11.163	1.00	0.52	1SG 501
ATOM	501		VAL	63	14.445	61.338	-12.394	1.00	0.52	1SG 502
ATOM	502	C	VAL	63	15.086	62.480	-9.863	1.00	0.52	1SG 503
ATOM	503	o	VAL	63	15.924	62.309	-8.980	1.00	0.52	15G 504
ATOM	504	N	ASN	64	15.146		-10.731	1.00	0.32	15G 505 18G 506
ATOM	505	CA	ASN	64	16.248		-10.842	1.00	0.32	15G 507
ATOM	506	CB	ASN	64	16.078		-12.013	1.00	0.32	15G 508
ATOM	507	ÇG	ASN	64	16.191	64.599	-13.303	1.00	0.32	15G 509
MOTA	508		asn	64	15.323		-13.630	1.00	0.32	15G 510
MOTA	509		asn	64	17.296	64.827 65.225	-14.062 -9.588	1.00	0.32	1SG 511
ATOM	510	C	ASN	64	16.425 17.531	65.680	-9.305	1.00	0.32	15G 512
ATOM	511	0	ASN	64 65	15.338	65.442	-8.825	1.00	0.25	1SG 513
ATOM	512	N	ASP	65	15.318	66.284	-7.655	1.00	0.25	15G 514
MOTA	513 514	CA CB	ASP ASP	65	13.909	66.571	-7.117	1.00	0.25	1SG 515
ATOM	515	CG	ASP	65	13.324	67.671	-7.985	1.00	0.25	1SG 516
ATOM ATOM	516		ASP	65	13.629	67.694	-9.207	1.00	0.25	1SG 517
ATOM	517		ASP	65	12.581	68.522	-7.428	1.00	0.25	15G 518
ATOM	518	c	ASP	65	16.143	65.782	-6.505	1.00	0.25	1SG 519
ATOM	519	Ö	ASP	65	16.459	66.561	-5.609	1.00	0.25	19G 520 1SG 521
ATOM	520	N	SER	66	16.465	64.481	-6.423	1.00	0.26	15G 522
ATOM	521	CA	SER	55	17.211	64.032	-5.275	1.00	0.26 0.26	1SG 523
ATOM	522	CB	SER	56	17.558	62.533	-5.309	1.00	0.26	1SG 524
MOTA	523	OG	SER	66	16.372	61.755	-5.255 -5.185	1.00	0.26	18G 525
MOTA	524	C	SER	66	18.509	64.781 65.300	-6.177	1.00	0.26	1SG 526
ATOM	525	0	SER	66	19.017 19.071	64.884	-3.958	1.00	0.35	1SG 527
MOTA	525	N	GLY	6 7 67	20.340	65.543	-3.821	1.00	0.35	1SG 528
MOTA	527	CA	GLY	67	20.318	66.412	-2.603	1.00	0.35	1SG 529
ATOM	528	C O	GLY	67	19.423	66.318	-1.765	1.00	0.35	1SG 530
ATOM	529	N	GLU	68	21.326	67.300	-2.473	1.00	0.40	1SG 531
ATOM	530 531	CA	GLU	68	21.354	68.137	-1.311	1.00	0.40	1SG 532
MOTA MOTA	532	CB	GLU	68	22.726	68.230	-0.620	1.00	0.40	1SG 533
ATOM	533	CG	GLU	68	23.845	68.792	-1.495	1.00	0.40	1SG 534
ATOM	534	CD	GLU	58	25.108	68.817	-0.647	1.00	0.40	1SG 535 1SG 536
ATOM	535		GLU	68	25.6 6 3	67.720	-0.373	1.00	0.40	15G 537
ATOM	536	OE2	GLU	68	25.528	69.937	-0.250	1.00	0.40	15G 538
ATOM	537	C	GLU	68	20.920	69.512	-1.698	1.00	0.40	15G 539
MOTA	538	0	GLU	68	21.211	69.986 70.173	-2.795 -0.796	1.00	0.34	1SG 540
ATOM	539	N	TYR	69	20.167 19.709	71.508	-1.056	1.00	0.34	1SG 541
ATOM	540	CA	TYR	69 69	18.186	71.508	-0.940	1.00	0.34	15G 542
MOTA	541	CB	TYR	69 69	17.520	71.002	-2.077	1.00	0.34	1SG 543
ATOM	542	CG	TYR	69	17.280	69.648	-2.029	1.00	0.34	1SG 544
MOTA	543		TYR	69	17.127	71.715		1.00	0.34	1SG 545
ATOM	544 545		TYR	69	16.661	69.014		1.00	0.34	1SG 546
ATOM	243	.								

ATOM	546	CE2	TYR	6 9	16.507	71.087	-4.240	1.00	0.34	15G 5 4 7
ATOM	547	CZ	TYR	69	16.275	69.733	-4.185	1.00	0.34	15G 548
ATOM	548	OH	TYR	69	15.639	69.084	-5.265	1.00	0.34	15G 549
ATOM	549	C	TYR	69	20.315	72.420	-0.037	1.00	0.34	1SG 550
ATOM	550	0	TYR	69	20.468	72.053	1.127	1.00	0.34	15G 551
ATOM	551	N	ARG	70	20.700	73.640	-0.46B	1.00	0.33	1SG 552
ATOM	552	CA	ARG	70	21.233	74.613	0.442	1.00	0.33	1SG 553
ATOM	553	СВ	ARG	70	22.767	74.627	0.507	1.00	0.33	1SG 554
ATOM	554	CG	ARG	70	23.309	73.406	1.253	1.00	0.33	1SG 555
ATOM	555	CD	ARG	70	24.830	73.388	1.424	1.00	0.33	1SG 556
ATOM	556	NE	ARG	70	25.431	72.997	0.119	1.00	0.33	1SG 557
ATOM	557	CZ	ARG	70	26.690	72.472	0.081	1.00	0.33	1SG 558
ATOM	558	NHl		70	27.408	72.344	1.235	1.00	0.33	1SG 559
ATOM	559	NH2		70	27.226	72.071	-1.108	1.00	0.33	1SG 560
ATOM	560	C	ARG	70	20.752	75.964	0.004	1.00	0.33	1SG 561
ATOM	561	ŏ	ARG	70	20.274	76.125	-1.117	1.00	0.33	1SG 562
ATOM	562	N	CYS	71	20.825	76.972	0.900	1.00	0.26	15G 563
ATOM	563	CA	CYS	71	20.377	78.289	0.535	1.00	0.25	15G 564
ATOM	564	CB	CYS	71	18.893	78.555	0.864	1.00	0.26	1 5G 565
ATOM	565	SG	CYS	71	18.496	78.615	2.636	1.00	0.26	1SG 566
ATOM	566	C	CYS	71	21.235	79.307	1.221	1.00	0.26	1SG 567
	567	0	CYS	71	21.949	78,991	2.172	1.00	0.26	15G 568
ATOM	568	N	GLN	72	21.215	80.559	0.711	1.00	0.14	1SG 569
MOTA		CA	GLN	72	22.005	B1.615	1.278	1.00	0.14	1SG 570
MOTA	569	СВ	GLN	72	23.405	81.712	0.643	1.00	0.14	1SG 571
ATOM	570	CG	GLN	72	24.303	82.785	1.260	1.00	0.14	1SG 572
ATOM	571	CD	GLN	72	25.638	82.750	0.528	1.00	0.14	15G 573
ATOM	572	OEI		72	25.792	82.069	-0.485	1.00	0.14	15G 574
MOTA	573	NE2	GLN	72	26.634	83.512	1.054	1.00	0.14	13G 575
MOTA	574	C	GLN	72	21.301	82.918	1.025	1.00	0.14	1SG 576
MOTA	575		GLN	72	20.515	83.054	0.087	1.00	0.14	1SG 577
ATOM	576	0	THR	73	21.576	83.916	1.892	1.00	0.15	1SG 578
MOTA	577	N		73	21.012	85.228	1.773	1.00	0.16	15G 579
ATOM	578	CA	THR THR	73 73	20.152	85.599	2.951	1.00	0.15	1SG 580
ATOM	579	CB		73	19.141	84.620	3.135	1.00	0.16	1SG 581
MOTA	580	OG1	THR	73 73	19.486	B6.959	2.679	1.00	0.16	1SG 582
ATOM	581	CG2	THR	73 73	22.191	86.155	1.737	1.00	0.16	1SG 583
ATOM	582	C	THR	73 73	23.325	85.730	1.942	1.00	0.16	15G 584
MOTA	583	0	THR	73 74	21.971	87.447	1.435	1.00	0.21	1SG 585
ATOM	584	N	ASN	74	23.072	88.368	1.377	1.00	0.21	1SG 586
ATOM	585	CA	ASN	74	22.697	89.763	0.849	1.00	0.21	1SG 587
ATOM	586	CB	ASN	74	22.617	89.670	-0.669	1.00	0.21	15G 588
ATOM	587	CG	asn Asn	74	22.270	90.635	-1.348	1.00	0.21	1SG 589
ATOM	588			74	22.961	88.475	-1.220	1.00	0.21	1SG 590
ATOM	589		asn asn	74	23.669	88.525	2.743	1.00	0.21	1 SG 591
ATOM	590 # 01	0	ASN	74	24.859	88.807	2.867	1.00	0.21	1SG 592
ATOM	591		LEU	7 5	22.825	88.433	3.790	1.00	0.22	18G 593
ATOM	592	N		75	23.180	88.556	5.181	1.00	0.22	1SG 594
ATOM	593	CA	LEU	75 75	21.987	88.944	6.070	1.00	0.22	1SG 595
ATOM	594	CB	LEU	75 75	21.434	90.348	5.763	1.00	0.22	15G 596
ATOM	595	CG	LEU	75 75	22.562	91.388	5.672	1.00	0.22	15G 597
ATOM	596		LEU	75 75	20.333	90.745	6.759	1.00	0.22	1SG 598
ATOM	597		LEU	75 75	23.804	87.324	5.785	1.00	0.22	1SG 599
ATOM	598	0	LEU	75 75	24.481	87.437	6.802	1.00	0.22	1SG 600
MOTA	599	0	LZU	75 76	23.574	86.107	5.251	1.00	0.32	1SG 601
ATOM	600	N	SER	76 76	24.037	84.956	5.989	1.00	0.32	1SG 602
ATOM	601	CA	SER		22.883	84.027	6.399	1.00	0.32	15G 603
ATOM	602	CB	SER	76 76	22.213	83.551	5.240	1.00	0.32	1SG 604
ATOM	503	O.C.	SER	76 76	25.017	84.125	5.215	1.00	0.32	1SG 605
MOTA	604	C	SER	76 76	25.282	84.360	4.038	1.00	0.32	1SG 606
ATOM	605	0	SER		25.634	83.142	5.909	1.00	0.43	1SG 507
MOTA	606	N	THR	77	23.034	JJ.142	3.303	1.00		

ATOM	607	CA	THR	77	26.525	82.222	5. 26 1	1.00	0.43	1SG 608
ATOM	608	СВ	THR	77	27.567	81.655	6.174	1.00	0.43	1 S G 609
ATOM	609	OG1	THR	7 7	25.955	80.928	7.228	1.00	0.43	1SG 610
ATOM	610	CGZ	THR	77	28.385	82.825	6.745	1.00	0.43	1SG 611
ATOM	611	C	THR	7 7	25.663	81.111	4.734	1.00	0.43	1SG 612
ATOM	612	ō	THR	7 7	24.471	81.058	5.032	1.00	0.43	1SG 613
ATOM	613	N	LEU	78	26.241	80.196	3.928	1.00	0.27	18G 614
ATOM	614	CA	LEU	78	25.474	79.156	3.293	1.00	0.27	1SG 615
ATOM	615	CB	LEU	78	26.307	78.312	2.309	1.00	0.27	1SG 616
MOTA	616	CG	LEU	78	25.499	77.245	1.545	1.00	0.27	1SG 617
ATOM	617		LEU	78	26.425	76.234	0.850	1.00	0.27	1SG 618
ATOM	618	CD1		78	24.498	77.891	0.572	1.00	0.27	1SG 619
ATOM	619	C	LEU	78	24.920	78.243	4.345	1.00	0.27	15G 620
ATOM	620	ō	LEU	78	25.581	77.931	5.333	1.00	0.27	15G 621
ATOM	621	N	SER	79	23.667	77.783	4.149	1.00	0.11	1SG 622
ATOM	622	CA	SER	79	23.037	76.937	5.124	1.00	0.11	1SG 623
ATOM	623	CB	SER	79	21.513	76.815	4.955	1.00	0.11	1SG 624
ATOM	624	QG	SER	79	21.213	76.083	3.776	1.00	0.11	1SG 625
ATOM	625	c	SER	79	23.595	75.557	5.010	1.00	0.11	1SG 626
ATOM	626	ō	SER	79	24.203	75.200	4.001	1.00	0.11	15G 627
ATOM	627	N	ASP	80	23.417	74.752	6.079	1.00	0.14	15G 628
ATOM	628	CA	ASP	80	23.841	73.383	6.047	1.00	0.14	18G 629
ATOM	629	СВ	ASP	80	23.747	72.664	7.406	1.00	0.14	15G 630
ATOM	630	CG	ASP	80	24.820	73.215	8.338	1.00	0.14	15G 631
MOTA	631		ASP	80	25.741	73.920	7.845	1.00	0.14	1SG 632
ATOM	632		ASP	80	24.733	72.931	9.562	1.00	0.14	15G 633
	633	C	ASP	80	22.908	72.703	5.097	1.00	0.14	15G 634
MOTA	634	o	ASP	80	21.786	73.158	4.880	1.00	0.14	1SG 635
ATOM	635	N	PRO	81	23.361	71.635	4.504	1.00	0.17	15G 63 6
ATOM	636	CA	PRO	81	22.566	70.959	3.515	1.00	0.17	1SG 637
MOTA	637	CD	PRO	81	24.783	71.457	4.267	1.00	0.17	15G 638
MOTA	638	CB	PRO	81	23.545	70.174	2.637	1.00	0.17	1SG 639
ATOM	639	CG	PRO	81	24.867	70.176	3.423	1.00	0.17	1SG 640
ATOM ATOM	640	C	PRO	81	21.445	70.127	4.045	1.00	0.17	1SG 641
MOTA	641	ò	PRO	81	21.508	69.669	5.185	1.00	0.17	1SG 642
ATOM	642	N	VAL	82	20.396	69.960	3.216	1.00	0.16	1SG 643
ATOM	643	CA	VAL	82	19.285	69.101	3.498	1.00	0.16	15G 644
ATOM	544	CB	VAL	82	17.965	59.817	3.475	1.00	0.15	1SG 645
ATOM	645		VAL	82	16.840	68.794	3.699	1.00	0.16	1SG 646
ATOM	645		VAL	82	18.008	70.940	4.524	1.00	0.16	1SG 647
ATOM	647	c	VAL	82	19.286	68.130	2.359	1.00	0.16	15G 648
ATOM	648	ō	VAL	82	19.289	68.539	1.198	1.00	0.16	1SG 649
ATOM	649	N	GLN	83	19.288	66.815	2.656	1.00	0.14	1SG 650
ATOM	650	CA	GLN	93	19.369	65.853	1.595	1.00	0.14	1SG 651
MOTA	651	ÇB	GLN	83	20.289	64.661	1.909	1.00	0.14	1SG 652
ATOM	652	CG	GLN	83	20.361	63.653	0.761	1.00	0.14	15G 653
ATOM	553	CD	GLN	83	21.289	62.516	1.166	1.00	0.14	15G 654
ATOM	654		GLN	83	21.088	61.372	0.761	1.00	0.14	1SG 655
ATOM	655		GLN	83	22.329	62.832	1.983	1.00	0.14	1SG 656
ATOM	656	С	GLN	83	18.000	65.310	1.325	1.00	0.14	1SG 657
ATOM	657	ō	GLN	83	17.265	64.946	2.241	1.00	0.14	1SG 658
ATOM	658	N	LEU	84	17.623	65.249	0.031	1.00	0.13	1SG 659
ATOM	659	CA	LEU	84	16.313	64.773	-0.309	1.00	0.13	1SG 660
ATOM	660	CB	LEU	84	15.463	65.842	-1.024	1.00	0.13	15G 661
ATOM	661	CG	LEU	84	14.045	65.379	-1.404	1.00	0.13	1SG 662
ATOM	662		LEU	84	13.376	66.379	-2.362	1.00	0.13	1SG 563
ATOM	663		LEU	84	13.193	65.093	-0.157	1.00	0.13	18G 664
ATOM	564	C	LEU	84	16.463	63.601	-1.234	1.00	0.13	190 665
ATOM	665	Ö	LEU	84	17.358	63.578	-2.077	1.00	0.13	15G 666
ATOM	666	N	GLU	85	15.609	62.565	-1.067	1.00	0.13	15G 667
ATOM	667	CA	GLU	85	15.659	61.442	-1.962	1.00	0.13	1SG 66 8

ATOM	668	CB	GLU	85	15.128	60.122	-1.323	1.00	0.13	1SG 669
ATOM	669	CG	GLU	85	17.623	60.111	-0.993	1.00	0.13	1SG 670
ATOM	670	CD	GLU	85	18.029	58.680	-0.573	1.00	0.13	15G 671
ATOM	671	OE1	GLU	85	17.391	58.068	0.224	1.00	0.13	15G 672
ATOM	672	OE2	GLU	85	18.980	58.178	-1.330	1.00	0.13	1SG 673
ATOM	673	C	GLU	85	14.284	61.216	-2.512	1.00	0.13	15G 674
ATOM	674	ō	GLU	85	13.323	61.034	-1.765	1.00	0.13	1SG 675
	675	N	VAL	86	14.161	61.211	-3.855	1.00	0.18	15G 676
MOTA	676	CA	VAL	86	12.880	61.025	-4.470	1.00	0.18	1SG 677
MOTA			VAL	86	12.628	61.986	-5.593	1.00	0.18	1SG 578
ATOM	677	CB		86	11.244	61.699	-6.195	1.00	0.18	1SG 679
ATOM	678	CG1	VAL		12.774	63.413	-5.038	1.00	0.18	1SG 680
ATOM	679	CG2	VAL	86		59.631	-5.014	1.00	0.18	15G 681
ATOM	680	c	VAL	86	12.831		-5.708	1.00	0.18	1SG 682
ATOM	681	0	VAL	86	13.746	59.188		1.00	0.34	1SG 683
atom	682	N	HIS	87	11.743	58.893	-4.710			15G 684
ATOM	683	CA	HIS	87	11.681	57.522	-5.133	1.00	0.34	
ATOM	684		HIS	87	13.107	57.437	-2.117	1.00	0.34	15G 685
ATOM	685	CG	HIS	87	12.856	56.525	-3.119	1.00	0.34	1SG 686
ATOM	686	CB	HIS	87	11.514	56.524	-3.963	1.00	0.34	15G 687
ATOM	687	NES	HIS	87	14.860	56.069	-2.186	1.00	0.34	1SG 688
MOTA	688	CD2	HIS	87	13.936	55.697	-3.147	1.00	0.34	15G 689
ATOM	689	CE1	HIS	87	14.318	57.118	-1.593	1.00	0.34	1SG 690
ATOM	690	С	HIS	87	10.467	57.302	-5.978	1.00	0.34	1SG 691
ATOM	691	0	HIS	87	9.539	58.109	-5.995	1.00	0.34	1SG 692
ATOM	692	N	ILE	88	10.485	56.205	-6.762	1.00	0.38	1SG 693
MOTA	693	CA	ILE	88	9.339	55.850	-7.542	1.00	0.38	1SG 694
ATOM	694	СВ	ILE	89	9.605	55.807	-9.024	1.00	0.38	15G 695
ATOM	695	CG2	ILE	88	10.824	54.912	-9.310	1.00	0.38	1SG 696
ATOM	696	CG1	ILE	88	8.323	55.418	-9.776	1.00	0.38	1SG 697
	697	CD1	ILE	88	8.409	55.623	-11.288	1.00	0.38	1SG 698
ATOM			ILE	88	8.899	54.495	-7.072	1.00	0.38	1SG 699
MOTA	698	C	ILE	88	9.501	53.472	-7.396	1.00	0.38	1SG 700
ATOM	699	0			7.809	54.464	-6.281	1.00	0.20	1SG 701
ATOM	700	N	GTA	89	7.304	53.227	-5.757	1.00	0.20	1SG 702
ATOM	701	CA	GLY	89	5.901	53.499	-5.315	1.00	0.20	15G 703
ATOM	702	Č	GLY	89	5.512		-5.141	1.00	0.20	15G 704
atom	703	0	GLY	89		54.651	-5.147	1.00	0.12	18G 705
ATOM	704	N	TRP	90	5.094	52.434	-4.750	1.00	0.12	1SG 706
ATOM	705	CA	TRP	90	3.723	52.586		1.00	0.12	1SG 707
ATOM	706	CB	TRP	90	2.880	51.313	-4.922	1.00	0.12	1SG 708
atom	707	CG	TRP	90	2.518	51.031	-6.358		0.12	18G 709
MOTA	708	CDS	TRP	90	1.448	51.700	-7.042	1.00	0.12	15G 710
atom	709	CD1	TRP	90	3.076	50.170	-7.258	1.00		15G 711
ATOM	710	NE1	TRP	90	2.414	50.255	-8.460	1.00	0.12	
ATOM	711	CEŻ	TRP	90	1.410	51.195	-8.341	1.00	0.12	1SG 712 1SG 713
ATOM	712	CE3	TRP	90	0.569	52.657	-5.619	1.00	0.12	
ATOM	713	CZ2	TRP	90	0.486	51.642	-9.241	1.00	0.12	15G 714
ATOM	714	CZ3	TRP	90	-0.361	53.107	-7.529	1.00	0.12	1SG 715
ATOM	715	CHZ	TRP	90	-0.400	52.508	-8.815	1.00	0.12	1SG 716
MOTA	716	C	TRP	90	3.580	53.037	-3.324	1.00	0.12	1SG 717
ATOM	717	0	TRP	90	2.663	53.800	-3.022	1.00	0.12	1SG 718
ATOM	718	N	LEU	91	4.446	52.560	-2.403	1.00	0.26	1SG 719
ATOM	719	CA	LEU	91	4.265	52.905	-1.015	1.00	0.26	1SG 720
ATOM	720	CB	LEU	91	3.562	51.776	-0.239	1.00	0.26	15G 721
ATOM	721	CG	LEU	91	3.157	52.126	1.203	1.00	0.26	1SG 722
ATOM	722		LEU	91	2.734	50.869	1.981	1.00	0.26	1SG 723
ATOM	723		LEU	91	2.079	53.222	1.222	1.00	0.26	1SG 724
ATOM	724	c	LEU	91	5.614	53.138	-0.385	1.00	0.26	1SG 725
ATOM	725	ō	LEU	91	6.577	52.431	-0.677	1.00	0.26	1SG 726
ATOM	726	N	LEU	92	5.719	54.138	0.522	1.00	0.38	1SG 727
ATOM	727	CA	LEU	92	6.998	54.439	1.103	1.00	0.38	1SG 728
ATOM	728	СВ	LEU	92	7.560	55.735	0.473	1.00	0.38	1SG 729
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MOTA	729	CG	LEU	92	9.071	56,015	0.609	1.00	0.38	1SG 730
MOTA	730		S TEA		9.558	55.970	2.057	1.00	0.38	15G 731
MOTA	731		L LEU		9.434	-	-0.076	1.00	0.38	1SG 732
ATOM	732	C	LEU	92	6.810		2.588	1.00	0.38	1SG 733
ATOM	733	0	LEU	92 93	5.768	55.108	3.043	1.00	0.38	15G 734
ATOM ATOM	734 735	N CA	LEU	93 93	7.804 7.741	54.221 54.488	3.402	1.00	0.28	18G 735
ATOM	736	CB	LEU	93	8.385	53.414	4.812 5.695	1.00	0.28	15G 736
ATOM	737	CG	LEU	93	8.272	53.774	7.184	1.00	0.28	1SG 737 1SG 738
ATOM	738		LEU	93	9.357	53.085	8.018	1.00	0.28	15G 739
ATOM	739		LEU	93	6.842	53.566	7.705	1.00	0.28	1SG 740
ATOM	740	C	LEU	93	8.566	55.725	5.002	1.00	0.28	1SG 741
MOTA	741	0	LEU	93	9.775	55.710	4.770	1.00	0.28	18G 742
ATOM	742	N	GLN	94	7.949	56.830	5.464	1.00	0.17	1SG 743
ATOM	743	CA	GLN	94	8.665	58.079	5.487	1.00	0.17	15G 744
ATOM	744	CB	GLN	94	7.823	59.244	4.936	1.00	0.17	1SG 745
ATOM ATOM	745 746	CD	GLN GLN	94 94	7.457	59.079	3.456	1.00	0.17	15G 746
ATOM	747		GLN	94	6.482 5.403	60.183	3.068 3.646	1.00	0.17	15G 747
ATOM	748	NE2		94	5.867	61.016	2.063	1.00	0.17 0.17	15G 748 15G 749
ATOM	749	C	GLN	94	9.119	58.445	6.869	1.00	0.17	15G 750
ATOM	750	Ö	GLN	94	8.489	58.092	7.864	1.00	0.17	1\$G 751
ATOM	751	N	ALA	95	10.270	59.157	6.949	1.00	0.22	1SG 752
ATOM	752	CA	ALA	95	10.807	59.602	8.209	1.00	0.22	15G 753
MOTA	753	CB	ALA	95	11.868	58.652	8.789	1.00	0.22	1SG 754
MOTA	754	C	ALA	95	11.466	60.944	8.020	1.00	0.22	1SG 755
MOTA	755	0	ALA	95	11.923	51.281	6.929	1.00	0.22	18G 756
ATOM	756	N	PRO	96	11.450	61.752	9.055	1.00	0.32	1SG 757
MOTA MOTA	757 758	CA	PRO	96 96	12.110		9.060	1.00	0.32	1SG 758
MOTA	759	CB	PRO	96	10.425 11.422	61.656 63.855	10.079 10.153	1.00	0.32	1SG 759 1SG 760
ATOM	760	CG	PRO	96	10.741	62.805	11.048	1.00	0.32	1SG 760 1SG 761
MOTA	761	c	PRO	96	13.591	62.923	9.280	1.00	0.32	15G 761
ATOM	762	ō	PRO	96	14.314	63.852	8.921	1.00	0.32	1SG 763
ATOM	763	N	ARG	97	14.065	61.820	9.898	1.00	0.53	1SG 764
MOTA	764	CA	ARG	97	15.473	51.698	10.174	1.00	0.53	1SG 765
ATOM	765	CB	ARG	97	15.898	62.263	11.541	1.00	0.53	1SG 766
ATOM	756	CG	ARG	97	15.826	63.783	11.675	1.00	0.53	13G 767
ATOM	767	CD	ARG	97	16.303	64.269	13.047	1.00	0.53	1SG 768
ATOM	768 769	NE CZ	ARG ARG	97 97	16.192	65.754	13.073	1.00	0.53	1SG 769
ATOM ATOM	770		ARG	97 97	15.441 15.772	66.436	14.229 15.367	1.00	0.53	1SG 770
ATOM	771	NH2		97	16.772	65.759 67.798	14.244	1.00	0.53 0.53	1SG 771 1SG 772
ATOM	772	C	ARG	97	15.838	60.245	10.235	1.00	0.53	15G 772
ATOM	773	ō	ARG	97	14.998	59.389	10.508	1.00	0.53	15G 774
ATOM	774	N	TRP	98	17.112	59.947	9.899	1.00	0.63	18G 775
ATOM	775	CA	TRP	98	17.708	58.639	9.981	1.00	0.63	1SG 776
MOTA	776	CB	TRP	98	19.044	58.563	9.225	1.00	0.63	15G 777
MOTA	777	CG	TRP	98	18.963	58.722	7.727	1.00	0.63	1 SG 778
ATOM	778		TRP	98	19.073	57.635	6.796	1.00	0.63	1SG 779
ATOM	7 7 9		TRP	98	18.829	59.858	5.982	1.00	0.63	1SG 780
ATOM ATOM	780 781	NE1 CEZ		98 98	18.849 19.000	59.546 58.181	5.644 5.515	1.00	0.63	1SG 781
ATOM	782	CE3		98	19.000	56.293	5.313 6.993	1.00	0.63	15G 782 1SG 783
ATOM	783	CZZ		98	19.083	57.388	4.406	1.00	0.63	1SG 784
ATOM	784	CZ3		98	19.308	55.495	5.873	1.00	0.63	1SG 785
ATOM	785	CH2		98	19.235	56.033	4.604	1.00	0.63	1SG 786
ATOM	786	С	TRP	98	18.054	58.309	11.401	1.00	0.63	1SG 787
MOTA	787	0	TRP	98	17.880	57.176	11.851	1.00	0.63	15G 788
MOTA	788	N	VAL	99	18.595	59.298	12.142	1.00	0.34	1SG 789
ATOM	789	CA	VAL	99	19.048	59.025	13.477	1.00	0.34	15G 790

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ATOM	790	CB	VAL	99	20.524	59.219	13.662	1.00	0.34	1SG 791
ATOM	791	CG1	VAL	99	20.863	58.957	15.139	1.00	0.34	15G 792
ATOM	792	CG2	VAL	99	21.271	58.304	12.576	1.00	0.34	15G 793
ATOM	793	C	VAL	99	18.367	59.959	14.419	1.00	0.34	15G 794
ATOM	794	0	VAL	99	18.049	61.095	14.072	1.00	0.34	1SG 795
ATOM	795	N	PHE	100	18.120	59.475	15.651	1.00	0.22	1SG 796
ATOM	796	CA	PHE	100	17.482	60.261	16.666	1.00	0.22	1SG 797
ATOM	797	CB	PHE	100	16.050	59.805	17.011	1.00	0.22	15G 798
ATOM	798	CG	PHE	100	15.147	60.050	15.850	1.00	0.22	1SG 799
ATOM	799	CD1	PHE	100	15.045	59.126	14.835	1.00	0.22	15G 800
ATOM	800		PHE	100	14.393	61.200	15.781	1.00	0.22	1SG 801
ATOM	801		PHE	100	14.210	59.348	13.765	1.00	0.22	15G 802
ATOM	802	CE2	PHE	100	13.557	51,428	14.714	1.00	0.22	1SG 803
ATOM	803	CZ	PHE	100	13.464	60.501	13.704	1.00	0.22	15G 804
ATOM	804	C	PHE	100	18.269	60.096	17.929	1.00	0.22	1\$G 805
ATOM	805	0	PHE	100	19.106	59.202	18.044	1.00	0.22	1SG 806
ATOM	806	N	LYS	101	18.022	60.982	18.914	1.00	0.37	1SG 807
ATOM	807	CA	LYS	101	18.685	60.871	20.179	1.00	0.37	1SG 808
ATOM	808	CB	LY5	101	19.121	62.219	20.781	1.00	0.37	15G 809
ATOM	809	CG	LYS	101	20.001	62.084	22.025	1.00	0.37	15G 810
ATOM	810	CD	LYS	101	20.705	63.381	22.431	1.00	0.37	1SG 811
ATOM	811	CE	LYS	101	21.583	63.228	23.674	1.00	0.37	15G 812
ATOM	812	NZ	LYS	101	20.740	62.951	24.858	1.00	0.37	1SG 813
ATOM	813	Ç	LYS	101	17.693	60.252	21.105	1.00	0.37	15G 814
MOTA	814	ŏ	LYS	101	16.495	60.245	20.827	1.00	0.37	1SG 815
ATOM	815	N	GLU	102	18.163	59.687	22.231	1.00	0.39	1SG 816
ATOM	816	CA	GLU	102	17.220	59.044	23.095	1.00	0.39	1SG 817
ATOM	817	CB	GLU	102	17.844	58.321	24.301	1.00	0.39	1SG 818
ATOM	818	CG	GLU	102	16.843	57.503	25.120	1.00	0.39	15G 819
ATOM	819	CD	GLU	102	17.615	56.757	26.198	1.00	0.39	18G 820
ATOM	820		GLU	102	18.311	57.431	27.003	1.00	0.39	15G 821
ATOM	821	OE2	GLU	102	17.521	55.500	26.228	1.00	0.39	15G 822
ATOM	822	Ċ	GLU	102	16.283	60.078	23.620	1.00	0.39	1SG 823
ATOM	823	ō	GLU	102	16.570	61.220	23.867	1.00	0.39	1SG 824
MOTA	824	N	GLU	103	15.011	59.670	23.799	1.00	0.36	1SG 825
ATOM	825	CA	GLU	103	13.964	60.488	24.342	1.00	0.36	15G 826
ATOM	826	CB	GLU	103	14.455	61.396	25.484	1.00	0.36	1SG 827
ATOM	827	CG	GLU	103	13.329	52.144	26.202	1.00	0.36	15G 828
ATOM	828	CD	GLU	103	13.884	62.673	27.516	1.00	0.36	1SG 829
ATOM	829	OE1		103	14.575	63.727	27.492	1.00	0.36	1SC 830
MOTA	830	OE2		103	13.629	62.021	28.564	1.00	0.36	1SG 831
ATOM	831	C	GLU	103	13.304	61.337	23.292	1.00	0.36	1SG 832
MOTA	832	ō	GLU	103	12.292	51.973	23.577	1.00	0.36	1SG 833
ATOM	833	N	ASP	104	13.805	61.348	22.040	1.00	0.43	15G 834
ATOM	834	CA	ASP	104	13.164	62.158	21.035	1.00	0.43	1SG 835
ATOM	835	СВ	ASP	104	14.062	62.472	19.824	1.00	0.43	1SG 836
MOTA	836	CG	ASP	104	15.128	53.467	20.261	1.00	0.43	1SG 837
ATOM	837	OD1	ASP	104	14.791	64.371	21.072	1.00	0.43	1SG 838
MOTA	838		ASP	104	16.289	63.343	19.786	1.00	0.43	1SG 839
ATOM	839	С	ASP	104	11.960	61.429	20.519	1.00	0.43	15G 840
ATOM	840	0	ASP	104	11.861	60.207	20.619	1.00	0.43	15G 841
ATOM	841	N	PRO	105	11.000	62.175	20.031	1.00	0.49	15G 84Z
ATOM	842	CA	PRO	105	9.848	61.540	19.444	1.00	0.49	15G 843
ATOM	843	CD	PRO	105	10.635	63.393	20.738	1.00	0.49	15G 844 15G 845
ATOM	844	CB	PRO	105	8.700	62.541	19.551	1.00	0.49	15G 845
ATOM	845	CG	PRO	105	9.098	63.424	20.745	1.00	0.49	
ATOM	846	С	PRO	105	10.124	61.111	18.035	1.00	0.49	15G 847
ATOM	847	0	PRO	105	10.660	61.908	17.264	1.00	0.49	1SG 848
ATOM	848	N	ILE	106	9.727	59.883	17.652	1.00	0.36	15G 849
ATOM	849	CA	ILE	106	9.943	59.473	16.295	1.00	0.36	15G 850 1SG 851
ATOM	850	CB	ILE	106	10.523	58.093	16.165	1.00	0.36	199 031

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ATOM	851	ÇG2	ILE	106	10.559	57.725	14.672	1.00	0.36	15G 85Z
ATOM	852	CG1	ILE	106	11.905	58.028	16.839	1.00	0.36	15G 853
ATOM	853	CD1	ILE	106	12.457	56.609	16.954	1.00	0.36	1SG 854
ATOM	854	C	ILE	106	8.601	59.479	15.637	1.00	0.36	15G 855
ATOM	855	0	ILE	105	7.648	58.886	16.143	1.00	0.36	15G 856
MOTA	856	N	HI5	107	8.487	60.185	14.495	1.00	0.24	1SG 857
ATOM	857	CA	HIS	107	7.250	60.266	13.772	1.00	0.24	15G 858
MOTA	858	ND1	HIS	107	5.419	61.664	11.375	1.00	0.24	1SG 859
ATOM	859	CG	HIS	107	5.521	61.800	12.741	1.00	0.24	15G 860 15G 861
MOTA	860	CB	HIS	107	6.811	61.712	13.496	1.00	0.24	15G 862
ATOM	861	NES	HIS	107	3.359	62.008	12.134	1.00	0.24	15G 863
ATOM	862	CD2		107	4.254	62.011	13.189	1.00	0.24	15G 864
ATOM	863		HIS	107	4.105	61.797	11.065	1.00	0.24	15G 865
ATOM	864	С	HIS	107	7.455	59.623	12.437	1.00	0.24	15G 866
MOTA	865	0	HIS	107	8.426	59.919	11.743	1.00	0.32	1SG 867
MOTA	866	N	LEU	108	6.532	58.728 58.051	10.776	1.00	0.32	1SG 868
ATOM	867	CA	LEU	108	6.678	56.568	10.770	1.00	0.32	1SG 869
ATOM	868	CB	LEU	108	7.053	56.337	11.629	1.00	0.32	15G 870
ATOM	869	CG	LEU	108	8. 4 01 9.528	57.138	10.963	1.00	0.32	19G 871
ATOM	870		LEU	108 108	8.722	54.838	11.741	1.00	0.32	1SG 872
ATOM	871		LEU	108	5.365	58.089	10.057	1.00	0.32	1SG 873
ATOM	872 873	0	LEU	108	4.317	58.287	10.669	1.00	0.32	1SG 874
MOTA	874	N	ARG	109	5.391	57.926	8.715	1.00	0.56	1SG 875
MOTA	875	CA	ARG	109	4.152	57.926	7.992	1.00	0.56	15G 876
MOTA MOTA	875	CB	ARG	109	3.759	59.308	7.445	1.00	0.56	1SG 877
ATOM	877	CG	ARG	109	2.437	59.292	6.678	1.00	0.56	15G 878
ATOM	878	CD	ARG	109	1.919	60.679	6.297	1.00	0.56	15G 879
ATOM	879	NE	ARG	109	2.988	61.367	5.522	1.00	0.56	15G 880
ATOM	880	CZ	ARG	109	2.734	61.825	4.262	1.00	0.56	15G 881
ATOM	881	NH1	ARG	109	1.540	61.554	3.664	1.00	0.56	15G 882
ATOM	882	NH2	ARG	109	3.674	62.558	3.597	1,00	0.56	1SG 883 1SG 884
ATOM	883	C	ARG	109	4.246	56.981	6.835	1.00	0.56 0.56	15G 885
ATOM	884	0	ARG	109	5.286	56.856	6.190	1.00	0.57	15G 886
ATOM	885	N	CZS	110	3.129	56.286	6.547	1.00	0.57	15G 887
MOTA	886	CA	CYS	110	3.049	55.357 54.160	5.458 5.827	1.00	0.57	15G 888
atom	887	CB	CYS	110	2.169 2.263	52.785	4.659	1.00	0.57	1SG 889
MOTA	888	SG	CYS	110	2.373	56.124	4.366	1.00	0.57	1SG 890
ATOM	889	C	CYS	110 110	1.224	56.532	4.524	1.00	0.57	1SG 891
ATOM	890	0	CYS HIS	111	3.069	56.339	3.228	1.00	0.38	1SG 892
MOTA	891	n Ca	HIS	111	2.538	57.210	2.212	1.00	0.38	1SG 893
ATOM ATOM	892 893		HIS	111	3.845	59.725	-0.098	1.00	0.38	1SG 894
MOTA	894	CG	HIS	111	3.026	59.397	0.958	1.00	0.38	1SG 895
MOTA	895	CB	HIS	111	3.431	58.454	2.048	1.00	0.38	15G 896
MOTA	896		HIS	111	1.950	60.848	-0.391	1.00	0.38	1SG 897
ATOM	897		HIS	111	1.872	60.091	0.765	1.00	0.38	15G 898
ATOM	898		HIS	111	3.153	60.597	-0.874	1.00	0.38	1SG 899
MOTA	899	C	HIS	111	2.419	56.523	0.884	1.00	0.38	15G 900
ATOM	900	0	HIS	111	3.335	55.837	0.435	1.00	0.38	1SG 901 1SG 902
ATOM	901	N	SER	112	1.273	56.736	0.198	1.00	0.32	15G 902
ATOM	902	CA	SER	112	1.044	56.101	-1.070	1.00	0.32	15G 904
ATOM	903	CB	SER	112	-0.389	55.569	-1.218	1.00	0.32	18G 905
ATOM	904	OG	SER	112	-0.492	54.787	-2.396 -2.172	1.00	0.32	15G 906
MOTA	905	Ç	SER	112	1.307	57.088 58.302	-2.1/2	1.00	0.32	1SG 907
ATOM	906	0	SER	112	1.242	56.569	-3.372	1.00	0.30	1SG 908
ATOM	907	N	TRP	113	1.638 1.963	57.399	-4.497	1.00	0.30	1SG 909
ATOM	908	CA	TRP	113 113	2.495	56.585	-5.697	1.00	0.30	1SG 910
MOTA	909	CB CG	TRP	113	2.901	57.379	-6.919	1.00	0.30	1SG 911
ATOM	910 911	CDZ		113	2.390	57.139	-8.240	1.00	0.30	1SG 912
ATOM	211	هر د	* ***		3.000					

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										1SG 913
s most	912	CD1	TRP	113	3.833	58.368			0.30	15G 914
ATOM	913		TRP	113	3.923	58.771			0.30 0.30	15G 915
MOTA	914		TRP	113	3.046	58.019				1SG 916
MOTA	915		TRP	113	1.459	56.252			0.30	15G 917
MOTA	916		TRP	113	2.778	58.026	-10.441		0.3 0 0.3 0	15G 918
ATOM	917	CZ3	TRP	113	1.187	56.267	-10.050		0.30	15G 919
atom Atom	918	CH2	TRP	113	1.834		-10.903		0.30	15G 920
ATOM ATOM	919	С	TRP	113	0.745	58.163	-4.905		0.30	1SG 921
ATOM	920	0	TRP	113	-0.351	57.617	-5.020	1.00	0.27	1SG 922
ATOM	921	N	LYS	114	0.922	59.482	-5.109	1.00	0.27	15G 923
ATOM	922	CA	LYS	114	-0.135	60.350	-5.539	1.00	0.27	15G 924
ATOM	923	CB	LYS	114	-0.677	59.986	-6.931	1.00	0.27	1SG 925
ATOM	924	CG	LY5	114	0.364	60.164	-8.037 - 9.375	1.00	0.27	1SG 926
ATOM	925	CD	LYS	114	-0.039	59.543		1.00	0.27	1SG 927
ATOM	926	CE	LYS	114	-0.974	60.429	-10.198	1.00	0.27	15G 928
ATOM	927	NZ	LYS	114	-1.297		-11.480 -4.557	1.00	0.27	1SG 929
ATOM	928	С	LYS	114	-1.266	60.310	-4.895	1.00	0.27	15G 930
ATOM	929	0	LYS	114	-2.398	60.652	-3.300	1.00	0.32	1SG 931
ATOM	930	N	ASN	115	-0.981	59.925	-2.258	1.00	0.32	1SG 932
ATOM	931	CA	ASN	115	-1.970	59.921 61.333	-1.958	1.00	0.32	15G 933
ATOM	932	CB	asn	115	-2.435	61.990	-1.078	1.00	0.32	18G 934
ATOM	933	ÇG	ASN	115	-1.305	61.364	-0.209	1.00	0.32	1SG 935
ATOM	934	OD1	ASN	115	-0.700	63.280	-1.391	1.00	0.32	15G 936
MOTA	935	NDZ		115	-1.011	59.118	-2.626	1.00	0.32	18G 937
ATOM	936	С	ASN	115	-3.177	59.534	-2.353	1.00	0.32	1SG 938 °
MOTA	937	0	ASN	115	-4.302	57.932	-3.236	1.00	0.37	1SG 939
MOTA	938	N	THR	116	-2.997 -4.165	57.141	-3.495	1.00	0.37	15G 940
ATOM	939	CA	THR	116	-3,909	55.918	-4.321	1.00	0.37	1SG 941
MOTA	940	CB	THR	116	-5.135	55.293	-4.672	1.00	0.37	18G 94Z
ATOM	941	061		116	-3.039	54.961	-3.497	1.00	0.37	1SG 943
ATOM	942	CG2		116 116	-4.668	56.703	-2.156	1.00	0.37	15G 944
MOTA	943	C	THR THR	116	-3.888	56.517	-1.222	1.00	0.37	15G 945 15G 946
MOTA	944	0	ALA	117	-5.996	56.517	-2.030	1.00	0.24	15G 947
ATOM	945	N CA	ALA	117	-6.570	56.202	-0.752	1.00	0.24	13G 948
MOTA	946	CB	ALA	117	-8.090	55.960	-0.804	1.00	0.24	15G 949
ATOM	947 948	C	ALA	117	-5.923	54.971	-0.212	1.00	0.24	1SG 950
MOTA	949	Ö	ALA	117	-5.750	53.980	-0.917	1.00	0.24	1SG 951
ATOM	950	N	LEU	118	-5.541	55.021		1.00	0.13	15G 952
MOTA MOTA	951	CA	LEU	118	-4.872	53.905		1.00	0.13	1SG 953
ATOM	952	CB	LEU	118	-3.382	54.199		1.00	0.13	15G 954
ATOM	953	ÇG	LEU	118	-2.589	53.047		1.00	0.13	15G 955
ATOM	954	CD	LEU	118	-1.222			1.00	0.13	18G 956
ATOM	955	CD	LEU	118	-2.469			1.00	0.13	1SG 957
ATOM	956	C	LEU	118	-5.514			1.00	0.13	1SG 958
ATOM	957	0	LEU	118	-5.848	-		1.00	0.15	1SG 959
ATOM	958	N	HIS	119	-5.714			1.00	0.15	15G 960
ATOM	959			119	-6.265			1.00	0.15	1SG 961
ATOM	960	ND.	1 HIS	119	-8.820 -8.548			1.00	0.15	15G 962
MOTA	961			119	-7.782				0.15	1SG 963
ATOM	962			119	-9.697				0.15	1SG 964
MOTA	963		2 HIS	119	-9.091 -9.091				0.15	1SG 965
ATOM	964		S HIZ	119	-9.508		-		0.15	15G 966
MOTA	965		1 HIS	119 119	-5.579				0.15	15G 967
ATOM	966		HI5	119	-4.75					15G 968
ATOM	967		HIS	120	-5.895					15G 969
MOTA	966		LYS	120	-5.32					15G 970 15G 971
MOTA	969				-5.71	47.72	6 5.981			
ATOM	970 970				-7.21	1 47.43	8 6.003			
ATOM	97.				-7.65	4 45.44	6 4.927	1.00	0.15	100 713
ATOM	3/4									

* MON	973	CE	LYS	120	-9.159	46.178	4.933	1.00	0.15	1SG 974
MOTA	974	NZ	LYS	120	-9.537	45.384	3.742	1.00	0.15	1SG 975
ATOM	975	C	LYS	120	-3.828	49.079	6.773	1.00	0.15	1SG 976
ATOM	975	0	LYS	120	-3.147	48.236	6.191	1.00	0.15	1SG 977
ATOM	-	N	VAL	121	-3.270	50.096	7.459	1.00	0.12	15G 978
ATOM	977		VAL	121	-1.847	50.293	7.458	1.00	0.12	1SG 979
ATOM	978	CA	VAL	121	-1.443	51.742	7.478	1.00	0.12	1SG 980
ATOM	979	CB	VAL	121	. 0.090	51.832	7.576	1.00	0.12	150 981
MOTA	980	CG1 CG2	VAL	121	-2.025	52.431	6.232	1.00	0.12	15G 982
ATOM	981	C	VAL	121	-1.240	49.648	8.662	1.00	0.12	15G 9B3
MOTA	982		VAL	121	-1.756	49.748	9.775	1.00	0.12	1SG 984
MOTA	983	0	THR	122	-0.115	48.932	8.447	1.00	0.20	15G 985
ATOM	984	N CA	THR	122	0.569	48.321	9.545	1.00	0.20	18G 986
MOTA	985		THR	122	0.565	46.820	9.506	1.00	0.20	15G 987
ATOM	986	CB CC1		122	-0.770	46.335	9,535	1.00	0.20	15G 988
MOTA	987	OG1	THR	122	1.344	46.294	10.725	1.00	0.20	1SG 989
MOTA	988	CG2	THR		1.993	48,778	9.503	1.00	0.20	1SG 990
ATOM	989	C	THR	122	2.590	48.895	8.433	1.00	0.20	15G 991
MOTA	990	0	THR	122	2.562	49.073	10.688	1.00	0.31	18G 992
MOTA	991	N	TYR	123	3.935	49.480	10.795	1.00	0.31	1SG 993
ATOM	992	CA	TYR	123 123	4.175	50.652	11.755	1.00	0.31	1SG 994
ATOM	993	CB	TYR		3.858	51.920	11.056	1.00	0.31	15G 995
MOTA	994	CG	TYR	123	2.569	52.379	10.913	1.00	0.31	1SG 996
MOTA	995		TYR	123 123	4.901	52.652	10.544	1.00	0.31	1SG 997
ATOM	996	CD2	TYR	123	2.334		10.261	1.00	0.31	15G 998
ATOM	997	CE1	TYR		4.673	53.835	9.896	1.00	0.31	15G 999
MOTA	998	CES	TYR	123	3.391	54.291	9.756	1.00	0.31	1SG1000
ATOM	999	CZ	TYR	123	3,181	55.511	9.089	1.00	0.31	1SG1001
ATOM	1000	OH	TYR	123	4.690	48.339	11.381	1.00	0.31	15G1002
ATOM	1001	C	TYR	123	4.273	47.754	12.386	1.00	0.31	1SG1003
MOTA	1002	0	TYR	123	5.843	47.994	10.770	1.00	0.32	15G1004
MOTA	1003	N	LEU	124	6.599	46.877	11.259	1.00	0.32	13G1005
ATOM	1004	CA	LEU	124	6.814	45.787	10.192	1.00	0.32	1SG1006
MOTA	1005	CB	LEU	124	5.515	45.183	9.624	1.00	0.32	15G1007
ATOM	1006	CG	LEU	124	4.590	44.673	10.739	1.00	0.32	15G1008
MOTA	1007		LEU	124	5.817	44.105	8.571	1.00	0.32	1SG1009
ATOM	1008		LEU	124	7.971	47.343	11.640	1.00	0.32	15G1010
MOTA	1009	C	LEU	124	8.523	48.248	11.017	1.00	0.32	1SG1011
ATOM	1010	0	LEU	124	8.543	46.757	12.714	1.00	0.33	1SG1012
ATOM	1011	Ŋ	GLN	125	9.913	47.045	13.032	1.00	0.33	15G1013
MOTA	1012	CA	GLN	125	10.152	47.788	14.359	1.00	0.33	1SG1014
ATOM	1013	CB	GLN	125	9.779	47.001	15.612	1.00	0.33	15G1015
atom	1014	CG	GLN	125	10.320	47.769	16.812	1.00	0.33	1SG1016
MOTA	1015	CD	GLN	125	11.527	47.814	17.044	1.00	0.33	15G1017
MOTA	1016		GLN	125	9.403	48.390	17.600	1.00	0.33	1SG1018
MOTA	1017	NE2		125	10.597	45.721	13.137	1.00	0.33	15G1019
MOTA	1018	C	GLN	125	10.185	44.856	13.907	1.00	0.33	15G1020
MOTA	1019	0	GLN	125	11.665	45.529	12.346	1.00	0.22	1SG1021
ATOM	1020	N	ASN	126	12.397	44.297	12.359	1.00	0.22	15G1022
ATOM	1021	CA	ASN	126	13.085	44.005	13.704	1.00	0.22	15G1023
ATOM	1022	CB	ASN	126	14.202	45.024	13.875	1.00	0.22	15G1024
ATOM	1023	CG	ASN	126 126	14.904	45.347	12.919	1.00	0.22	15G1025
MOTA	1024		ASN		14.369	45.551	15.118	1.00	0.22	1SG1026
ATOM	1025		ASN		11.473	43.152	12.041	1.00	0.22	15G1027
MOTA	1026	Ċ	ASN		11.685	42.036	12.491	1.00	0.22	15G1028
MOTA	1027	0	ASN		10.420		11.245	1.00	0.15	1 SG1 029
MOTA	1028	N	GLY		9.558	42.371	10.800	1.00	0.15	1SG1030
ATOM	1029	CA	GLY		8.459		11.784	1.00	0.15	15G1031
ATOM	1030	C	GLY		7.651		11.556	1.00	0.15	1SG1032
MOTA	1031	0	GLY LYS		8.386		12.907	1.00	0.28	1SG1033
ATOM	1032	N	LYS		7.305		13.827	1.00	0.28	1SG1034
MOTA	1033	CA	פנע							

ATOM	1034	CB	LYS	128	7.745	42.359	15.281	1.00	0.28	1SG1035
MOTA	1035	CĠ	LYS	128	5.576	41.990	16.198	1.00	0.28	1SG1036
MOTA	1036	CD	LYS	128	5.995	41.432	17.55B	1.00	0.28	15G1037
ATOM	1037	CE	LYS	128	7.294	42.514	18.598	1.00	0.28	15G1038
ATOM	1038	NZ	LYS	128	7.675	41.886	19.883	1.00	0.28	1SG1039
ATOM	1039	C	LYS	128	6.427	43.808	13.822	1.00	0.28	15G1040
ATOM	1040	0	LYS	128	6.920	44.933	13.880	1.00	0.28	1SG1041
ATOM	1041	N	ASP	129	5.092	43.604	13.758	1.00	0.47	1SG1042
ATOM	1042	CA	ASP	129	4.182	44.713	13.654	1.00	0.47	1SG1043
ATOM	1043	CB	ASP	129	2.781	44.323	13.141	1.00	0.47	15G1044
ATOM	1044	CG	ASP	129	2.148	43.334	14.108	1.00	0.47	15G1045
ATOM	1045		ASP	129	2.903	42.693	14.887	1.00	0.47	1501046
ATOM	1046		ASP	129	0.896	43.199	14.070	1.00	0.47	19G1047
ATOM	1047	C	ASP	129	4.040	45.423	14.954	1.00	0.47	1SG1048
ATOM	1048	ō	ASP	129	3.732	44.821	15.991	1.00	0.47	15G1049
ATOM	1049	N	ARG	130	4.370	46.733	14.954	1.00	0.54	1SG1050
ATOM	1050	CA	ARG	130	4.239	47.624	16.073	1.00	0.54	1SG1051
ATOM	1051	CB	ARG	130	5.171	48.845	15.964	1.00	0.54	1SG1052
ATOM	1052	CG	ARG	130	5.312	49.632	17.271	1.00	0.54	15G1053
ATOM	1053	CD	ARG	130	4.047	50.382	17.689	1.00	0.54	1SG1054
ATOM	1054	NE	ARG	130	4.325	51.062	18.984	1.00	0.54	1SG1055
ATOM	1055	CZ	ARG	130	3.388	51.032	19.976	1.00	0.54	15G1056
ATOM	1056		ARG	130	2.230	50.330	19.800	1.00	0.54	15G1057
ATOM	1057		ARG	130	3.612	51.697	21.147	1.00	0.54	13G1058
MOTA	1058	С	ARG	130	2.835	48.152	16.192	1.00	0.54	1SG1059
ATOM	1059	0	ARG	130	2.308	48.302	17.293	1.00	0.54	1SG1060
ATOM	1060	N	LYS	131	2.196	48.478	15.048	1.00	0.34	15G1061
MOTA	1061	CA	LYS	131	0.921	49.141	15.109	1.00	0.34	1SG1062
MOTA	1062	CB	LYS	131	1.106	50.668	15.097	1.00	0.34	1SG1063
ATOM	1063	CG	LYS	131	-0.168	51.511	15.150	1.00	0.34	1SG1064
ATOM	1064	CD	LYS	131	0.143	53.009	15.235	1.00	0.34	1SG1065
ATOM	1065	CE	LYS	131	-1.058	53.916	14.962	1.00	0.34	15G1066
ATOM	1066	NZ	LYS	131	-0.665	55.338	15.068	1.00	0.34	13G1067
ATOM	1067	C	LYS	131	0.121	48.809	13.888	1.00	0.34	15G1068
ATOM	1068	ō	LYS	131	0.657	48.725	12.784	1.00	0.34	15G1069
ATOM	1069	N	TYR	132	-1.202	48.610	14.067	1.00	0.18	1SG1070
ATOM	1070	CA	TYR	132	-2.078	48.392	12.952	1.00	0.18	1SG1071
ATOM	1071	CB	TYR	132	-2.580	46.941	12.832	1.00	0.18	15G1072
ATOM	1072	ĊG	TYR	132	-3.692	46.919	11.840	1.00	0.18	1 S G1073
MOTA	1073		TYR	132	-3.441	46.903	10.488	1.00	0.18	1SG1074
ATOM	1074	CD2	TYR	132	-4.999	46.936	12.267	1.00	0.18	1 SG 1075
ATOM	1075		TYR	132	-4.474	46.888	9.581	1.00	0.18	15G1076
ATOM	1076	CE2	TYR	132	-6.037	46.920	11.364	1.00	0.18	1SG1077
ATOM	1077	CZ	TYR	132	-5.774	46.893	10.016	1.00	0.18	15G1078
ATOM	1078	OH	TYR	132	-6.827	46.877	9.078	1.00	0.18	15G1079
ATOM	1079	C	TYR	132	-3.270	49.277	13.136	1.00	0.18	15G1080
ATOM	1080	0	TYR	132	-3.826	49.344	14.229	1.00	0.18	1SG1081
ATOM	1081	N	PHE	133	-3.674	50.009	12.073	1.00	0.16	15G1082
ATOM	1082	CA	PHE	133	-4.842	50.847	12.146	1.00	0.16	1SG1083
ATOM	1083	CB	PHE	133	-4.561	52.324	12.491	1.00	0.15	15G1084
MOTA	1084	CG	PHE	133	-4.409	52.420	13.969	1.00	0.15	15G1085
ATOM	1085	CD1	PHE	133	-3.262	51.996	14.596	1.00	0.15	1SG1086
ATOM	1086	CD2	PHE	133	-5.424	52.951	14.731	1.00	0.16	15G1087
ATOM	1087	CEl	PHE	133	-3.140	52.090	15.962	1.00	0.16	15G1088
MOTA	1088	CEZ	PHE	133	-5.307	53.049	15.097	1.00	0.16	1SG1089
ATOM	1089	CZ	PHE	133	-4.161	52.615	16.716	1.00	0.16	1 5 G1090
ATOM	1090	С	PHE	133	-5.527	50.820	10.821	1.00	0.16	15G1091
ATOM	1091	0	PHE	133	-4.886	50.846	9.774	1.00	0.16	15G1092
ATOM	1092	N	HIS	134	-6.869	50.736	10.828	1.00	0.26	15G1093
MOTA	1093	CA	HIS	134	-7.547	50.719	9.569	1.00	0.26	15G1094
MOTA	1094	ND1	HIS	134	-9.410	47.923	9.166	1.00	0.26	1\$G1095

ATOM	1095	CĠ	HIS	134	-9.255	48.944	10.077	1.00	0.26	13G1096
ATOM	1096	CB	HIS	134	-9.039	50.378	9. 69 7	1.00	0.26	1SG1097
ATOM	1097	NE2		134	-9.537	46.998	11.184	1.00	0.25	15G1098
ATOM	1098	CD2		134	-9.334	48.361	11.304	1.00	0.25	15G1099
ATOM	1099	CEL		134	-9.576	46.782	9.881	1.00	0.26	1SG1100
ATOM	1100	С	HIS	134	-7.425	52.058	8.902	1.00	0.26	1SG1101
ATOM	1101	0	HIS	134	-7.150	52.143	7.709	1.00	0.26	1SG1102
ATOM	1102	N	HIS	135	-7.712	53.138	9.650	1.00	0.40	15G1103
ATOM	1103	CA	HIS	135	-7.716	54.478	9.124	1.00	0.40	1SG1104
ATOM	1104	ND1		135	-8.378	55.032	12.360	1.00	0.40	15G1105 15G1106
ATOM	1105	CG	HIS	135	-8.228	55.796	11.224	1.00	0.40	15G1107
MOTA	1106	CB	HIS	135	-8.708	55.391	9.862	1.00	0.40	15G1108
ATOM	1107	NE2		135	-7.321	56.889	12.977	1.00	0.40	1SG1109
atom	1108	-	HIS	135	-7.581	56.926 55.733	11.619 13.379	1.00	0.40	1SG1110
ATOM	1109		HIS	135	-7.818 -5.411	55.226	9.122	1.00	0.40	1SG1111
ATOM	1110	C C	HIS	135 135	-6.136	55.962	8.176	1.00	0.40	1SG1112
ATOM	1111	0	HIS	136	-5.579	55.078	10.177	1.00	0.34	1SG1113
ATOM	1112	N	ASN	136	-4.497	56.015	10.365	1.00	0.34	15G1114
ATOM	1113	CA	nea Nea	136	-4.255	56.339	11.847	1.00	0.34	1 SG 1115
ATOM	1114	CB	ASN	136	-3.317	57.529	11.904	1.00	0.34	15 G11 16
ATOM	1115		ASN	136	-2.170	57.400	12.325	1.00	0.34	15G1117
atom Atom	1116 1117		ASN	136	-3.806	58.715	11.451	1.00	0.34	15G1118
ATOM	1118	C	ASN	136	-3.187	55.580	9.769	1.00	0.34	15G1119
ATOM	1119	ō	ASN	136	-2.653	54.518	10.075	1.00	0.34	1SG1120
ATOM	1120	N	SER	137	-2.651	56.454	8.892	1.00	0.23	1SG1121
ATOM	1121	CA	SER	137	-1.429	56.362	8.136	1.00	0.23	1SG1122
ATOM	1122	CB	SER	137	-1.431	57.298	6.916	1.00	0.23	1SG1123
ATOM	1123	OG	SER	137	-2.479	56.939	6.028	1.00	0.23	15G1124
ATOM	1124	С	SER	137	-0.202	56.706	8.943	1.00	0.23	1SG1125
ATOM	1125	0	SER	137	0.906	56.514	8.445	1.00	0.23	15G1126
ATOM	1126	N	ASP	138	-0.334	57.310	10.147	1.00	0.21	15G1127 15G1128
ATOM	1127	CA	ASP	138	0.853	57.763	10.837	1.00	0.21	15G1128
ATOM	1128	CB	ASP	138	0.793	59.245	11.273	1.00	0.21 0.21	1SG1130
ATOM	1129	ÇG	ASP	138	-0.332	59.471	12.281	1.00	0.21	15G1131
MOTA	1130		ASP	138	-0.325	58.810	13.354	1.00	0.21	1SG1132
ATOM	1131		ASP	138	-1.221	60.313	11.986 12.047	1.00	0.21	1\$G1133
MOTA	1132	C	ASP	138	1.179	56.931 56.172	12.550	1.00	0.21	1SG1134
MOTA	1133	0	A5P	138 139	2.442	57.061	12.525	1.00	0.22	18G1135
ATOM	1134	N Ca	PHE	139	2.972	56,316	13.635	1.00	0.22	1SG1136
ATOM	1135	CA	PHE	139	3.793	55.124	13.104	1.00	0.22	15G1137
ATOM	1136 1137	CB	PHE	139	4.421	54.316	14.186	1.00	0.22	15G1138
ATOM	1138	CD1		139	3.664	53.563	15.055	1.00	0.22	1SG1139
ATOM ATOM	1139		PHE	139	5.792	54.273	14.287	1.00	0.22	15G1140
ATOM	1140		PHE	139	4.270	52.812	16.034	1.00	0.22	15G1141
	1141		PHE	139	6.404	53.523	15.263	1.00	0.22	1SG1142
ATOM ATOM	1142	cz	PHE	139	5.640	52.793	15.141	1.00	0.22	1SG1143
ATOM	1143	C	PHE	139	3.858	57.225	14.441	1.00	0.22	15G1144
ATOM	1144	ō	PHE	139	4.645	57. 99 2	13.885	1.00	0.22	1SG1145
ATOM	1145	N	HIS	140	3.748	57.165	15.789	1.00	0.24	15G1146
ATOM	1146	CA	HIS	140	4.541	58.034	16.620	1.00	0.24	15G 114 7 15G1 14 8
ATOM	1147	ND1	HIS	140	1.861	59.659	15.668	1.00	0.24	15G1149
ATOM	1148	CG	HIS	140	2.970	60.039	16.391	1.00	0.24	1SG1149 1SG1150
MOTA	1149	CB	HIS	140	3.716	59.128	17.321	1.00	0.24	1SG1150
ATOM	1150		HIS	140	2.223	61.801	15.196	1.00	0.24	15G1152
ATOM	1151		HIS	140	3.178	61.350	16.090 14.970	1.00	0.24	15G1153
MOTA	1152		HIS	140	1.455 5.125	60.750 57.228	17.739	1.00	0.24	1SG1154
ATOM	1153	Ċ	HIS	140	4.444	56.404	18.347	1.00	0.24	1SG1155
ATOM	1154	0	HIS	140	6.419	57.455	18.041	1.00	0.25	1\$G1156
MOTA	1155	N	ILE	141	0.473	31.400	70.047			- · · · · - ·

									0 35	1SG1157
ATOM	1156	CA	ILE	141	7.045	56.791	19.144	1.00	0.25	15G1157
MOTA	1157	CB	ILE	141	8.257	56.002	18.742	1.00	0.25	15G1159
ATOM	1158	CG2	ILE	141	8.889	55.427	20.020	1.00	0.25	
ATOM	1159	CG1	ILE	141	7.895	54.928	17.704	1.00	0.25	15G1160
ATOM	1160	CD1	ILE	141	9.115	54.309	17.023	1.00	0.25	1SG1161
ATOM	1161	С	ILE	141	7.531	57.873	20.052	1.00	0.25	1SG1162
ATOM	1162	0	ILE	141	8.477	58.587	19.723	1.00	0.25	1SG1163
ATOM	1163	N	PRO	142	6.892	58.036	21.175	1.00	0.43	1SG1164
ATOM	1164	CA	PRO	142	7.352	59.024	22.107	1.00	0.43	1SG1165
	1165	CD	PRO	142	5.453	57.854	21.248	1.00	0.43	1 5G 1166
ATOM	1166	CB	PRO	142	6.139	59.430	22.947	1.00	0.43	1SG1167
ATOM			PRO	142	5.083	58.350	22.652	1.00	0.43	15G1168
MOTA	1167	CG		142	8.466	58.424	22.902	1.00	0.43	15G1169
ATOM	1168	C	PRO		8.482	57.204	23.054	1.00	0.43	1SG1170
ATOM	1169	0	PRO	142	9.387	59.260	23.422	1.00	0.52	1SG1171
ATOM	1170	N	LYS	143		58.801	24.241	1.00	0.52	15G1172
MOTA	1171	CA	LYS	143	10.473		25.651	1.00	0.52	15G1173
MOTA	1172	CB	LYS	143	10.025	58.371		1.00	0.52	15G1174
MOTA	1173	CG	LYS	143	9.356	59.483	26.461	1.00	0.52	18G1175
ATOM	1174	CD	LY5	143	10.243	60.707	26.696		0.52	15G1176
MOTA	1175	CE	LYS	143	9.553	61.806	27.508	1.00		1SG1177
ATOM	1176	NZ	LYS	143	8.346	62.283	26.794	1.00	0.52	
ATOM	1177	C	LYS	143	11.135	57.616	23.605	1.00	0.52	1SG1178
ATOM	1178	0	LYS	143	10.991	56.492	24.083	1.00	0.52	1SG1179
ATOM	1179	N	ALA	144	11.886	57.840	22.508	1.00	0.40	15G1180
ATOM	1180	CA	ALA	144	12.533	56.758	21.817	1.00	0.40	15G1181
ATOM	1181	CB	ALA	144	13.097	57.155	20.441	1.00	0.40	15G1182
ATOM	1182	c	ALA	144	13.672	56.228	22.636	1.00	0.40	1SG1183
	1183	ŏ	ALA	144	14.282	56.947	23.427	1.00	0.40	1SG1184
MOTA	1184	N	THR	145	13.981	54.926	22.444	1.00	0.44	15G1185
ATOM	1185	CA	THR	145	15.003	54.249	23.191	1.00	0.44	1SG1186
MOTA		CB	THR	145	14.400	53.346	24.239	1.00	0.44	1SG1187
ATOM	1186		THR	145	13.520	54.104	25.056	1.00	0.44	1SG1188
ATOM	1187	0G1	THR	145	15.497	52.747	25.138	1.00	0.44	15G1189
ATOM	1188	CG3		145	15.788	53.422	22.200	1.00	0.44	15G1190
MOTA	1189	C	THR		15.482	53.410	21.010	1.00	0.44	15G1191
MOTA	1190	0	THR	145		52.724	22.675	1.00	0.63	1SG1192
ATOM	1191	N	LEU	145	16.840	51.323	21.890	1.00	0.63	1SG1193
MOTA	1192	CA	LEU	146	17.739	51.319	22.739	1.00	0.63	15G1194
ATOM	1193	CB	LEU	146	18.871		23.396	1.00	0.63	1SG1195
ATOM	1194	ÇĞ	LEU	145	19.780	52.375	23.988	1.00	0.63	1SG1196
ATOM	1195		LEU	146	21.044	51.733		1.00	0.63	1SG1197
ATOM	1196	CD1	LEU	146	19.008	53.219	24.424		0.63	15G1198
ATOM	1197	C	LEU	145	17.007	50.780	21.252	1.00	0.63	1SG1199
MOTA	1198	0	LEU	146	17.373	50.337	20.165	1.00	0.64	15G1200
ATOM	1199	N	LYS	147	15.970	50.250	21.924	1.00		1SG1201
MOTA	1200	CA	LYS	147	15.234	49.124	21.415	1.00	0.64	15G1202
ATOM	1201	CB	LYS	147	14.155	48.611	22.381	1.00	0.64	
ATOM	1202	CG	LYS	147	14.737	47.990	23.651	1.00	0.64	15G1203
ATOM	1203	CD	LYS	147	15.708	46.838	23.378	1.00	0.64	15G1204
ATOM	1204	CE	LYS	147	15.081	45.661	22.626	1.00	0.64	1SG1205
ATOM	1205	NZ	LYS	147	15.060	45.938	21.172	1.00	0.64	15G1206
ATOM	1206	Ċ	LYS	147	14.553	49.511	20.138	1.00	0.64	1SG1207
ATOM	1207	o	LYS	147	14.327	48.669	19.271	1.00	0.64	1SG1208
	1208	N	ASP	148	14.198	50.802	20.011	1.00	0.39	15G1209
ATOM ATOM	1209	CA	ASP	148	13.491	51.371	18.897	1.00	0.39	15G1210
	1210	CB	ASP	148	13.077	52.834	19.134	1.00	0.39	15G1211
MOTA	1211	CG	ASP	148	11.977	52.847	20.187	1.00	0.39	15G1212
MOTA			ASP	148	11.064	51.984	20.096	1.00	0.39	1SG1213
ATOM	1212		ASP ASP	148	12.030	53.724	21.090	1.00	0.39	1SG1214
ATOM	1213				14.314	51.324	17.639	1.00	0.39	1\$G1215
ATOM	1214	Č	ASP	148	13.763	51.464	16.551	1.00	0.39	1SG1216
MOTA	1215	0	ASP	148	15.653	51.209	17.725	1.00	0.24	19G1217
MOTA	1216	N	SER	149	23.033	52.205				

N COLOM	1217	CA	SER	149	16.434	51.189	16.513	1.00	0.24	1SG1218
ATOM		СВ	SER	149	17.948	51.047	16.748	1.00	0.24	19G1Z19
ATOM	1218	OG	SER	149	18.448	52.160	17.471	1.00	0.24	15G1220
MOTA	1219		SER	149	16.031	49.996	15.702	1.00	0.24	15G1221
ATOM	1220	C		149	15.620	48.977	16.252	1.00	0.24	1SG1222
ATOM	1221	0	SER		16.118	50.089	14.354	1.00	0.24	1SG1223
ATOM	1222	N	GLY	150		48.914	13.596	1.00	0.24	1SG1224
ATOM	1223	CA	GLY	150	15.795	49,283	12.229	1.00	0.24	15G1225
MOTA	1224	С	GLY	150	15.308		11.818	1.00	0.24	1SG1226
MOTA	1225	0	GLY	150	15.351	50.442	11.485	1.00	0.20	1501227
MOTA	1226	N	SER	151	14.819	48.268	10.149	1.00	0.20	15G122B
MOTA	1227	CA	SER	151	14.351	48.492		1.00	0.20	15G1229
ATOM	1228	CB	SER	151	14.691	47.344	9.185		0.20	1SG1230
MOTA	1229	OG	SER	151	15.099	47.212	9.061	1.00	0.20	15G1231
ATOM	1230	С	SER	151	12.862	48.605	10.193	1.00		15G1232
ATOM	1231	0	SER	151	12.174	47.715	10.692	1.00	0.20	15G1232
ATOM	1232	N	TYR	152	12.327	49.722	9.661	1.00	0.35	1SG1234
ATOM	1233	CA	TYR	152	10.906	49.925	9.663	1.00	0.35	1SG1235
ATOM	1234	CB	TYR	152	10.463	51.277	10.254	1.00	0.35	
ATOM	1235	CG	TYR	152	10. 6 39	51.246	11.735	1.00	0.35	1SG1236
ATOM	1236	CD1		152	11.873	51.440	12.314	1.00	0.35	15G1237
ATOM	1237	CD2	TYR	152	9.549	51.036	12.550	1.00	0.35	1SG1238
	1238	CEL	TYR	152	12.015	51.412	13.682	1.00	0.35	1SG1239
ATOM	1239	CE2	TYR	152	9.685	51.007	13.917	1.00	0.35	15G1240
MOTA		CZ	TYR	152	10.921	51.195	14.485	1.00	0.35	15G1241
MOTA	1240		TYR	152	11.068	51.168	15.887	1.00	0.35	15G1242
MOTA	1241	OH		152	10.384	49.868	8.258	1.00	0.35	15G1243
ATOM	1242	C	TYR	152	11.039	50.319	7.319	1.00	0.35	15G1244
MOTA	1243	O.	TYR		9.174	49.282	8.100	1.00	0.75	1SG1245
ATOM	1244	N	PHE	153	8.500	49.142	6.835	1.00	0.75	15G1246
MOTA	1245	CA	PHE	153	8.423	47.706	6.276	1.00	0.75	1SG1247
ATOM	1246	CB	PHE	153		46.992	6.083	1.00	0.75	15G1248
ATOM	1247	CG	PHE	153	9.717		7.151	1.00	0.75	15G1249
MOTA	1248		PHE	153	10.350	45.400	4.828	1.00	0.75	15G1250
ATOM	1249	CDZ	PHE	153	10.267	46.861		1.00	0.75	1SG1251
ATOM	1250	CEl		153	11.531	45.716	6.977	1.00	0.75	15G1252
MOTA	1251	CE2	PHE	153	11.445	46.177	4.647		0.75	1SG1253
MOTA	1252	CZ	PHE	153	12.083	45.607	5.724	1.00	0.75	18G1254
ATOM	1253	С	PHE	153	7.044	49.335	7.134	1.00	0.75	1SG1255
ATOM	1254	0	PHE	153	6.626	49.319	8.292	1.00	0.86	1SG1256
ATOM	1255	N	CY5	154	6.226	49.481	6.071	1.00	0.86	18G1257
ATOM	1256	CA	CY5	154	4.807	49.626	6.230	1.00		1SG1258
ATOM	1257	CB	CYS	154	4.356	51.084	6.045	1.00	0.86	15G1259
ATOM	1258	SG	CYS	154	2.557	51.224	5.915	1.00	0.86	1SG1250
ATOM	1259	С	CYS	154	4.117	48.817	5.167	1.00	0.86	1SG1261
ATOM	1260	0	CYS	154	4.680	48.544	4.108	1.00	0.86	15G1262
ATOM	1261	N	ARG	155	2.870	48.380	5.451	1.00	0.56	
ATOM	1262	CA	ARG	155	2.050	47.690	4.499	1.00	0.56	1SG1263
ATOM	1263	CB	ARG	155	1.825	46.206	4,836	1.00	0.56	15G1264
ATOM	1264	CG	ARG	155	3.105	45.370	4.777	1.00	0.56	1SG1265
ATOM	1265	CD	ARG	155	2.895	43.891	5.109	1.00	0.56	1SG1266
	1266	NE	ARG		2.510	43.797	6.545	1.00	0.56	1SG1267
ATOM	1267	CZ	ARG	155	1.952	42.646	7.022	1.00	0.56	1SG1268
ATOM			ARG		1.743	41.593	6.180	1.00	0.56	1SG1269
ATOM	1268		ARG		1.603	42.548	8.338	1.00	0.56	1SG1270
ATOM	1269				0.716	48.370	4.543	1.00	0.56	1SG1271
ATOM	1270	C	ARG		0.343	48.942	5.569	1.00	0.56	1SG1272
MOTA	1271	0	ARG		-0.028	48.351	3.416	1.00	0.35	1SG1273
ATOM	1273	N	GLY		-1.322	48.985	3.400	1.00	0.35	15G1274
MOTA	1273	CA	GLY		-2.002	48.544	2.110	1.00	0.35	15G1275
ATOM	1274	Ċ	GLY		-1.354	48.263	1.135	1.00	0.35	15G1276
ATOM	1275	0	GLY			48.794	2.057	1.00	0.37	18G1277
MOTA	1276	N	LEU		-3.344	48.734	0.841	1.00	0.37	15G1278
ATOM	1277	CA	LEU	157	-4.007	40.431	0.041		- -	=

ATOM	1278	CB	LEU	157	-5.300	47.603	1.002	1.00	0.37	1SG1279
ATOM	1279	CG	LEU	157	-6.516	48.389	1.183	1.00	0.37	1SG1280
ATOM	1280	CD2	LEU	157	-6.549	49.386	2.345	1.00	0.37	1SG1281
ATOM	1281	CD1	LEU	157	-7.805	47.425	1.325	1.00	0.37	15G1282
ATOM	1282	¢	LEU	157	-4.334	49.668	0.075	1.00	0.37	1SG1283
ATOM	1283	0	LEU	157	-4.844	50.650	0.612	1.00	0.37	15G1284
ATOM	1284	N	VAL	158	-3.984	49.648	-1.223	1.00	0.25	15G1285
ATOM	1285	CA	VAL	158	-4.299	50.717	-2.117	1.00	0.25	15G1286
ATOM	1286	CB	VAL	158	-3.125	51.171	-2.929	1.00	0.25	1SG1287
ATOM	1287	CG1	VAL	158	-3.625	52.124	-4.027	1.00	0.25	15G1288
ATOM	1288	CGZ	VAL	158	-2.088	51.796	-1.981	1.00	0.25	1SG1289
ATOM	1289	С	VAL	158	-5.279	50.130	-3.065	1.00	0.25	15G1290
ATOM	1290	0	VAL	158	-4.985	49.143	-3.738	1.00	0.25	1SG1291
ATOM	1291	N	GLY	159	-6.481	50.718	-3.149	1.00	0.14	15G1292
ATOM	1292	CA	GLY	159	-7.440	50.118	-4.018	1.00	0.14	1SG1293
MOTA	1293	C	GLY	159	-7.690	48.744	-3.485	1.00	0.14	1SG1294
MOTA	1294	0	GLY	159	-8.016	48.562	-2.315	1.00	0.14	15G1295
ATOM	1295	N	SER	160	-7.597	47.751	-4.385	1.00	0.21	15G1296
MOTA	1296	CA	SER	160	-7.836	46.363	-4.117	1.00	0.21	15G1297
ATOM	1297	CB	SER	160	-8.189	45.585	-5.397	1.00	0.21	13G1298
ATOM	1298	OG	SER	160	-9.399	46.082	-5.951	1.00	0.21	15G1299
MOTA	1299	С	SER	160	-6.697	45.631	-3.469	1.00	0.21	15G1300
ATOM	1300	0	SER	160	-6.940	44.695	-2.707	1.00	0.21	1SG1301
ATOM	1301	N	LYS	161	-5.428	45.995	-3.753	1.00	0.33	15G1302
MOTA	1302	CA	LYS	161	-4.384	45.112	-3.306	1.00	0.33	15G1303
ATOM	1303	CB	LYS	151	-3.423	44.675	-4.426	1.00	0.33	15G1304
ATOM	1304	CG	LY5	161	-4.077	43.773	-5.475	1.00	0.33	1SG1305
ATOM	1305	CD	LYS	161	-3.228	43.568	-6.732	1.00	0.33	15G1306
ATOM	1306	CE	LYS	161	-2.135	42.511	-6.567	1.00	0.33	15G1307
ATOM	1307	NZ	LYS	1 61	-1.386	42.355	-7.833	1.00	0.33	1SG1308
MOTA	1308	C	LYS	161	-3.550	45.700	-2.217	1.00	0.33	1SG1309
ATOM	1309	0	LY5	161	-3.514	46.909	-1.998	1.00	0.33	1SG1310
ATOM	1310	N	asn	162	-2.847	44.800	-1.499	1.00	0.32	1SG1311
ATOM	1311	CA	ASN	162	-1.996	45.168	-0.406	1.00	0.32	15G1312
ATOM	1312	CB	asn	162	-1.860	44.057	0.653	1.00	0.32	15G1313
MOTA	1313	CG	ASN	162	-0.975	44.545	1.794	1.00	0.32	15G1314
ATOM	1314	OD1		162	0.206	44.834	1.613	1.00	0.32	1SG1315
MOTA	1315		ASN	162	-1.568	44.637	3.015	1.00	0.32	1SG1316
MOTA	1316	C	ASN	162	-0.634	45.444	-0.958	1.00	0.32	15G1317 15G1318
MOTA	1317	0	ASN	162	-0.169	44.764	-1.872	1.00	0.32	15G1319
ATOM	1318	N	VAL	163	0.037	45.480	-0.419	1.00	0.27	15G1320
ATOM	1319	CA	VAL	163	1.352	46.811	-0.881	1.00	0.27	1SG1321
ATOM	1320	CB	VAL	163	1.412	48.149	-1,564	1.00	0.27	15G1321
ATOM	1321	CG1		163	2.865	48.442	-1.971	1.00	0.27	15G1323
MOTA	1322		VAL	163	0.427	48.136	-2.746	1.00	0.27	15G1323
ATOM	1323	C	VAL	163	2.256	46.869	0.311	1.00	0.27	1SG1325
MOTA	1324	0	VAL	163	1.803	47.074		1.00	0.29	15G1326
MOTA	1325	N	SER	164	3.568	46.544	0.088		0.29	15G1320
MOTA	1326	CA	SER	164	4.521	46.731	1.157	1.00	0.29	18G1328
MOTA	1327	CB	SER	164	5.214	45.401	1.489	1.00	0.29	1SG1329
ATOM	1328	oG	SER	164	6.044	45.006	0.409 0.728	1.00	0.29	15G1330
ATOM	1329	C	SER	164	5. 591 5.981	47.688 47.717	-0.438	1.00	0.29	15G1331
ATOM	1330	0	SER	164 165	5.981	48.513	1.672	1.00	0.29	15G1332
MOTA	1331	N	SER		7.106	49.478	1.365	1.00	0.20	15G1333
MOTA	1332	CA	SER SER	165 165	7.100	50.750	2.228	1.00	0.20	18G1334
MOTA	1333 1334	CB OG	SER SER	165	7.351	50.442	3.577	1.00	0.20	15G1335
ATOM	1335	C	SER	165	8.449	48.865	1.516	1.00	0.20	15G1336
MOTA MOTA	1335	0	SER	165	8.562	47.791	2.206	1.00	0.20	1SG1337
ATOM	1337	N	GLÜ	166	9.514	49.538	1.134	1.00	0.24	15G1338
ATOM	1338	ĊA	GLU	166	10.849	49.081	1.386	1.00	0.24	15G1339
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					44 000	4D 637	0.405	1.00	0.24	1SG1340
ATOM	1339	CB	GLU	166	11.899	49.631	-1.022	1.00	0.24	15G1341
ATOM	1340	CG	GLU	166	11.737	49.101	-1.884	1.00	0.24	15G1342
ATOM	1341	CD	GLU	166	12.830	49.716	-1.432	1.00	0.24	1SG1343
ATOM	1342	oe1	GLU	156	14.005	49.735	_	1.00	0.24	15G1344
ATOM	1343	OE2	GLU	156	12.500	50.180	-3.009 2.758	1.00	0.24	1SG1345
MOTA	1344	C	GLU	166	11.199	49.563		1.00	0.24	15G1346
MOTA	1345	0	GLU	166	10.560	50.471	3.286		0.37	15G1347
ATOM	1346	N	THR	167	12.223	48.948	3.382	1.00	0.37	15G1348
ATOM	1347	CA	THR	167	12.579	49.311	4.726	1.00	0.37	15G1349
ATOM	1348	CB	THR	167	13.348	48.260	5.469	1.00		15G1350
ATOM	1349	OG1	THR	167	13.474	48.621	6.836	1.00	0.37	15G1351
ATOM	1350	CG2	THR	167	14.741	48.133	4.831	1.00	0.37	15G1352
ATOM	1351	C	THR	167	13.464	50.514	4.734	1.00	0.37	15G1353
ATOM	1352	0	THR	167	14.103	50.863	3.742	1.00	0.37	1SG1354
ATOM	1353	N	VAL	168	13.478	51.191	5.899	1.00	0.32	15G1355
ATOM	1354	CA	VAL	168	14.342	52.301	6.161	1.00	0.32	1501356
ATOM	1355	CB	VAL	168	13.619	53.606	6.332	1.00	0.32	1SG1357
ATOM	1356		VAL	168	14.652	54.707	6.628	1.00	0.32	15G1358
ATOM	1357	CG2	VAL	168	12.777	53.870	5.071	1.00	0.32	15G1359
ATOM	1358	C	VAL	168	14.985	51.983	7.477	1.00	0.32	1SG1359
MOTA	1359	ō	VAL	168	14.311	51.562	8.417	1.00	0.32	1SG1361
MOTA	1360	N	ASN	169	16.315	52.167	7.582	1.00	0.27	
ATOM	1361	CA	ASN	159	16.961	51.845	8.820	1.00	0.27	15G1362
	1362	CB	ASN	169	18.405	51.332	8.659	1.00	0.27	1SG1363
ATOM	1363	CG	ASN	169	19.251	52.419	8.010	1.00	0.27	15G1364
ATOM	1364		ASN	169	18.923	52.927	5.93 9	1.00	0.27	1SG1365
MOTA	1365		ASN	169	20.374	52,794	B.680	1.00	0.27	15G1366
ATOM	1366	C	ASN	169	16.998	53.089	9.640	1.00	0.27	1SG1367
ATOM	1367	Ö	ASN	169	17.465	54.135	9.191	1.00	0.27	1SG1368
ATOM	1368	N	ILE	170	16.466	52.999	10.872	1.00	0.18	1SG1369
MOTA		CA	ILE	170	16.432	54.120	11.759	1.00	0.18	15G1370
ATOM	1369		ILE	170	15.039	54.499	12.169	1.00	0.18	1SG1371
ATOM	1370	CB	ILE	170	15.125	55.597	13.239	1.00	0.18	1SG1372
MOTA	1371		ILE	170	14.219	54.903	10.933	1.00	0.18	15G1373
MOTA	1372			170	12.736	55.115	11.224	1.00	0.18	15G1374
MOTA	1373		ILE	170	17.174	53.727	12.987	1.00	0.18	18G1375
MOTA	1374	C	ILE	170	16.957	52.654	13.549	1.00	0.18	15G1376
MOTA	1375	0	ILE		18.089	54.595	13.443	1.00	0.23	1SG1377
ATOM	1376	N	THR	171	18.828	54.212	14.600	1.00	0.23	1SG1378
MOTA	1377	CA	THR	171	20.303	54.095	14.351	1.00	0.23	15G1379
MOTA	1378	CB	THR	171	20.555	53.121	13.348	1.00	0.23	15G13B0
MOTA	1379		THR	171	20.992	53.691	15.665	1.00	0.23	1SG1381
MOTA	1380	CG2		171	18.633	55.238	15.658	1.00	0.23	15G1382
MOTA	1381	C	THR	171	18.599	56.440	15.396	1.00	0.23	15G1383
MOTA	1382	0	THR	171	18.448	54.760	16.899	1.00	0.52	13G1384
ATOM	1383	N	ILE	172	18.446	55.666	17.987	1.00	0.52	15G1385
ATOM	1384	CA	ILE	172	17.615	55.233	19.175	1.00	0.52	15G1386
MOTA	1385	CB	ILE	172	-	53.833	19.655	1.00	0.52	15G1387
ATOM	1386	CG2	ILE	172	18.032	56.325	20.257	1.00	0.52	15G1388
MOTA	1387	CG1	ILE	172	17.636 16.588	56.119	21.349	1.00	0.52	15G1389
MOTA	1388		ILE	172	19.882	55.716	18.301	1.00	0.52	15G1390
ATOM	1389	C	ILE	172	20.463	54.767	18.833	1.00	0.52	15G1391
ATOM	1390	0	ILE	172		56.859	17.933	1.00	0.62	15G1392
ATOM	1391	N	THR	173	20.493	57.061	18.114	1.00	0.62	18G1393
ATOM	1392	CA	THR	173	21.892	58.461	17.796	1.00	0.62	15G1394
MOTA	1393	CB	THR	173	22.335	58.461	17.821	1.00	0.52	1SG1395
ATOM	1394		LTHR		23.752		18.825	1.00	0.62	1501396
MOTA	1395	CG			21.728	59.430	19.551	1.00	0.62	1SG1397
ATOM	1396	С	THR		22.118	56.823	19.331	1.00	0.62	15G1398
MOTA	1397	0	THR		23.170	56.335		1.00		1SG1399
ATOM	1398	N	GLN		21.099	57.144				1SG1400
MOTA	1399		GLN	174	21.327	56.893	21.735	1.00	0.55	1000000

ATOM 1403 OE1 GLN 174 21.278 59.575 23.917 1.00 0.51 ATOM 1404 NE2 GLN 174 22.579 58.237 25.212 1.00 0.51 ATOM 1405 C GLN 174 21.464 55.387 21.896 1.00 0.51 ATOM 1406 O GLN 174 20.520 54.662 21.485 1.00 0.51 ATOM 1407 OXT GLN 174 22.513 54.940 22.435 1.00 0.51 END	15G1404 15G1405 15G1406 15G1407 15G1408	0.51 0.51 0.51	1.00 1.00 1.00 1.00	25.212 21.896 21.485	58.237 55.387 54.662	22.579 21.464 20.520	174 174 174	GLN GLN GLN	NE2 C O	. 1404 1405 1406	ATOM ATOM ATOM ATOM
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The following examples are provided for the purposes of illustration and are not intended to limit the scope of the present invention.

5 EXAMPLES

Example 1

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This example describes the construction of a recombinant baculovirus expressing soluble $Fc\gamma RIIa$ protein and the production of such protein.

Recombinant molecule pFcyRIIa, containing a nucleic acid molecule encoding a soluble form of human FcyRII (sFcyRIIa) operatively linked to baculovirus polyhedron transcription control sequences was produced as follows. The nucleic acid molecule sFcyRIIa was polymerase chain reaction (PCR) amplified from about 10 nanogram (ng) of FcyRIIaLR cDNA (described in detail in Ierino, et al., J. Exp. Med., vol. 178, pp. 1617-1628, 1993) using about 100 ng of primer NR1 having the nucleic acid sequence 5'-TAC GAA TTC CTA TGG AGA CCC AAA TGT CTC-3' (denoted SEQ ID NO:1) and primer FI2 having the nucleic acid sequence 50-CAT TCT AGA CTA TTG GAC AGT GAT GGT CAC-3' (denoted SEQ ID NO:2), using standard PCR methods. The resulting PCR 510 base pairs (referred to herein as product is sFcyRIIa(a)) and encodes the amino acid sequence represented herein by SEQ ID NO:3. Based on the results obtained in the Mass Spectroscopy experiment described in Example 7, a second protein product is present upon expression of a recombinant molecule comprising a PCR product of this Example. This data suggests that two PCR products were produced from the present method. The second PCR product is predicted to be 513 base pairs (referred to herein as sFcyRIIa(b)) and encodes the amino acid sequence represented herein by SEQ ID NO:12. The PCR products were digested with restriction endonucleases EcoRI and XbaI and ligated into unique EcoRI and XbaI sites of pVL1392

baculovirus shuttle plasmid (available from Pharmingen, San Diego, CA) to produce recombinant molecules referred to herein as pVL-sFcyRIIa(a) and pVL-sFcyRIIa(b).

recombinant molecules pVL-sFcvRIIa(a) pVL-sFcyRIIa(b) were co-transfected with baculovirus strain (available from Pharmingen) into Spodoptera frugiperda 21 (Sf-21) cells (available from Invitrogen San Diego, CA) to produce Corp., frugiperda:pVL-sFcyRIIa(a)/sFcyRIIa(b) cells. recombinant virus isolates were selected by screening on X-galactosidase plates for occlusion of b-galactosidase. Selected isolates were grown on monolayers of Sf-21 cells for infection using serum-free Sf900-II media (available from Gibco, New York) and the supernatant harvested about 40 hours post-infection. The presence of recombinant protein, referred to herein as PsFcyRIIa, supernatants was determined by ELISA using anti-FcyRII monoclonal antibodies 8.26 and 8.7 (described in detail in Ierino, et al., ibid.) using standard methods. the results described in Example 7, recombinant protein PsFcyRIIa includes the two species of protein having SEQ ID NO:3 and SEQ ID NO:12.

Example 2

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This example describes the purification of PsFcyRIIa for crystallization of the protein.

Supernatant from S. frugiperda: pVL-sFcyRIIa(a)/ sFcyRIIa(b) cells described above in Example 1 was harvested and then centrifuged at about x2000 rpm to remove Supernatant from the centrifugation was cellular debri. concentrated about five-fold using а Minitan^a ultrafiltration system (available from Millipore, Bedford, and then extensively dialyzed against a buffer containing 10 mM Tris-HCl pH 8.5, and 50 mM NaCl. dialyzed solution was applied to a Q-Sepharose fast-flow ion exchange column (available from Pharmacia, Uppsala,

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Sweden). The column was washed with 10 mM Tris-HCl, pH 8.5, and then protein was eluted from the column using a salt gradient from about of 0 to about 500 mM NaCl, passed over the column over 4 hours. PsFcyRIIa was eluted from the column at approximately 150 mM NaCl. The partially purified product was dialyzed against a buffer containing 20 mM Tris-HCl pH 7.4, and 30 mM NaCl. The dialysate was applied to a HAGG immuno-affinity chromatography column (described in detail in Ierino, et al., ibid.). The column was washed with a buffer containing 20 mM Tris-HCl pH 7.4, and 30 mM NaCl. PsFcyRIIa was eluted from the column using a buffer containing 0.1 M sodium acetate pH 4.0, and 0.5 M $\,$ The eluant was neutralized using 3m Tris pH8.0 and the dialysed against PBS (3.5 mM $NaH_2PO_42H_2O_7$, 16 mM Na_2HPO_4 , 150 mM NaCl). The dialysate was then concentrated approximately fifty-fold using macro and nanosep-10 ultra-filtration concentration devices (available from Filtron, Northborough, MA) and the applied to a G75 Superdex filtration column equilibrated in gel (available from Pharmacia, Uppsala, Sweden). Filtered PsFcyRIIa was dialyzed against 1 mM Tris-HCl pH 7.4 and concentrated to about 6 milligram per milliliter (mg/ml) of protein using macro and nanosep-10 ultra-filtration concentration devices. The purity of PsFcyRIIa was assessed by resolving the concentrated protein by SDS-PAGE and staining the protein with crocein scarlet. An electronic scan of the resulting gel is shown in Fig. 1, in which lane A contains supernatant harvested from a S. frugiperda:pVL-sFcyRIIa(a)/sFcyRIIa(b) cell culture prior to the ion-exchange step, lane B contains protein eluted from the affinity column, lane C contains protein isolated from the gel filtration chromatography step and lane D contains a sample of the PsFcyRIIa concentrated to 6 mg/ml and that was used for further crystallization studies. molecular weight markers are shown on the left side of the

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figure. The results indicate that the purified PsFcyRIIa was about 90% pure with apparent molecular weights of 25,000 daltons.

Example 3

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This example describes two-dimensional non-equilibrium pH gel electrophoresis analysis of purified PsFcyRIIa.

Supernatant from S. frugiperda:pVL-sFcyRIIa(a)/ sFcyRIIa(b) was incubated with about 20 microliter (ml) of packed Sepharose 4B beads conjugated with F(ab') fragments of anti-FcyRII monoclonal antibody 8.26 (IgG2b) production of which is described in J. Immunol., vol. 150, pp. 1-10, 1993) for about 1 hour at 4°C. The beads were then washed with buffer containing 10 mM Tris-HCl pH 7.4, 2% wt/vol bovine serum albumin (available from Commonwealth Serum Laboratories, Melbourne, Australia), 1 mM PMSF (available from Sigma Chemical Co., St. Louis, MO), 0.1% vol/vol Aprotinin (available from Sigma Chemical Co.), and then with 10 mM Tris-HCl, pH 7.4. The beads were resuspended in isoelectric about 50 ml focusing denaturation buffer (9.5 M urea, 4% acrylamide, 2% wt/vol NP-40, 2% total ampholines and 50 mM dithiothreitol), spun at about x13,000 rpm for about 2 minutes, loaded onto 4% tube gels and overlaid with about 10 ml of overlay buffer (9 M urea, 1% total ampholines) and anode buffer (0.01 M phosphoric acid), and electrophoresed for about 5 hours at about 550 Volts. The gels were then removed from the glass tubes, equilibrated in SDS-PAGE sample buffer (62.5 mM Tris-HCl, pH 6.8, 50 mM dithiothreitol and 10% glycerol) for about 2 hours at room temperature and attached to the top of a 13% slab gel for SDS-PAGE.

The electrophoresed proteins were transferred to Immobilon-P PVDF membrane (available from Millipore) using a semi-dry transfer cell (Biorad, Australia) under a 20 mA current for about 30 minutes. The membrane was blocked in PBS buffer containing 5% wt/vol skim milk for about 1 hour.

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The membrane was then incubated overnight with a rabbit anti-FcyRII polyclonal antisera (diluted 1:10,000 in PBS containing 5% wt/vol skimmilk) and then washed extensively with buffer (10 mM Tris-HCl, pH 8.0, 150 mM NaCl, 0.05% Tween-20). The polyclonal antisera was raised in rabbits by immunization with recombinant FcYRII protein. The animals were immunized with about 1 mg of FcyRII protein. For the first immunization, FcyRII protein was emulsified in complete Freunds adjuvant. Subsequent immunizations were performed using FcyRII protein emulsified in incomplete The membrane was then incubated with Freunds adjuvant. peroxidase-linked swine anti-rabbit antisera (available from Dako Corp., Denmark) (diluted 1:5000 in 10 Tris-HCl, pH 8.0, 150 mM NaCl and 0.05% Tween-20) for about 1 hour at room temperature. The membrane was washed before detection of the transferred protein using the enhanced (available Amersham from chemiluminescence system International, Australia).

An electronic scan of the resulting gels are shown in Figs. Fig. 2A illustrates the migration of protein 2A and 2B. supernatant harvested isolated from frugiperda:pVL-sFcyRIIa(a)/sFcyRIIa(b) cell cultures after Fig. 2B illustrates the migration of protein 34 hours. harvested from s.supernatant from isolated frugiperda:pVL-sFcyRIIa(a)/sFcyRIIa(b) cell cultures after The molecular weight markers are shown on the 73 hours. left side of the figure. The results indicate that the purified PsFcyRIIa has an apparent molecular weight of 25,000 daltons and a pI at about pH 6.

30 Example 4

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This example describes N-terminal peptide sequence of PsFcyRIIa.

Amino acid sequencing of purified PsFcyRIIa described in Example 2 using standard sequential Edman degradation method using an Applied Biosystem 470A gas phase sequenator

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coupled to an Applied Biosystem 130 separation system for automatic on-line analysis of the first eight amino acids (available from Applied Biosystems, CA). The n-terminal sequence was determined to be Ala-Pro-Pro-Lys-Ala-Val-Leu-Lys (denoted as SEQ ID NO:4).

Example 5

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This example describes the binding of PsFc γ RIIa to monomeric immunoglobulin.

Analysis of the interaction between PsFcyRIIa and monomeric immunoglobulin was performed using a BIAcore* 2000 biosensor (available from Pharmacia Biotech, Uppsala, Sweden) at about 22°C in Hepes buffered saline (HBS; 10 mM Hepes [N-2-hydroxyethylpiperazine-N'-2-ethanesulfonic acid, available from Commonwealth Serum Laboratories, Parkville, Australia], pH 7.4, 150 mM NaCl, 3.4 mM EDTA and 0.005% Surfactant, available from Pharmacia). About 4000 to about 6000 response units (RU) of monomeric human immunoglobulin subclasses IgG1, IgG2, IgG3, and IgE ($50\mu g/ml$ of each) were covalently coupled to separate carboxymethylated dextran surface of each CM5 sensor-chips (available from BIAcore, Uppsala, Sweden) using a amine coupling kit (available from BIAcore), according to manufacturer's methods. A series of PsFcyRIIa concentrations (about 0.001 to about 1 mg/ml protein) was injected over each sensor-chip surface for about 1 minute at about 20 μ l/min followed by about 3 minute dissociation phase. Following administration of the protein, the immunoglobulin surface was regenerated on each chip using a buffer containing 50 mM diethylamine pH 11.5, and 1 M NaCl. The equilibrium dissociation constants (K_{D}) for the interaction between PsFcyRIIa and immunoglobulin were obtained by non-linear curve fitting of a single site binding equation [Bound RU = $(B1_{max}.C)/(K_{D1} + C)$]; or a two site binding equation [Bound RU = ((B1_{max}.C)/(K_{D1} + C)) + $((B2_{max}.C)/(K_{D2} + C))]$, where $(B1_{max}$ refers to the maximum binding capacity of the surface at site 1; $B2_{\text{max}}$ refers to

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the maximum binding capacity of the surface at site 2; C refers to the concentration of PsFcyRIIa) and by linear curve fitting to Scatchard plots. Data points obtained from the IgE channels were subtracted to correct for refractive index differences. Data points between 50 and 60 seconds were averaged to obtain the amount of PsFcyRIIa bound at equilibrium for each PsFcyRIIa concentration.

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To determine the specificity of the interaction between PsFc γ RIIa and immobilized immunoglobulin, the interaction between PsFc γ RIIa with monomeric immunoglobulin was inhibited by the presence of excess monomeric IgG (Sandaglobulin, available from Sandoz, Basel, Switzerland). Using a fixed, half maximal dose of PsFc γ RIIa (50 μ g/ml), increasing concentrations of monomeric IgG (0 to 2 mg/ml IgG) were mixed with the PsFc γ RIIa, at about 22°C for about 1 hour before passing the PsFc γ RIIa over a sensor-chip surface coated with IgG1.

The results indicated that the binding of PsFcyRIIa to IgG3 and IgG1 was saturable over a broad range of protein concentrations. The maximum response units per protein concentration were plotted against the molar concentration of protein and curve fitting analyses undertaken. curve of best fit suggests that there are two regions of PsFcyRIIa that interact with IgG3. At 50% of the sites, the affinity for IgG3 was about $2.7 \times 10^6 M^{-1}$ and at the remaining 50% of the sites the affinity was about 1.2 x 10^4 M^{-1} (Fig. 3A). The interaction between PsFcyRIIa and IgG1 also occurred in two regions but the interaction was different from IgG3. Moreover, at about 90% of the ligand binding sites, the affinity of PsFcyRIIa for IgG1 was about 2.1 x $10^6 M^{-1}$ and at the remaining 10% of sites the affinity was about 2.3 x $10^4 M^{-1}$ (Fig. 3B). The interaction was specific for PsFcyRIIa since a six-fold molar excess of IgG completely inhibited binding of PsFcyRIIa to IgG. Analysis

of IgG2 binding was also performed and a Kd value of about 8 x $10^{-5}M^{-1}$ was obtained (Fig. 3C).

Example 6

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This example describes crystallization and X-ray diffraction of PsFcyRIIa.

A. Production of crystalline PsFcyRIIa

A series of alternative buffers were used to attempt to produce crystals of PsFcyRIIa by hanging drop vapor diffusion. Table 6 summarizes the different mother-liquor formulations used and the results obtained.

Table 6. Mother-liquor conditions and results of crystallization trial 3 mg/ml PsFcyRIIa.

	No.	SALT	BUFFER	PRECIPITANT*	рН	RESULT
	1	0.2M Calcium Chloride	0.1 M Acetate	30% MPD	4.6	clear drop
5	2			0.4M Na K Tartrate		fine precipitation
	3			0.4M Amm. Phosphate		clear drop
	4		0.1M Tris	2.0M Amm. Sulphate	8.5	clear drop
	5	0.2M Sodium Citrate	0.1M Hepes	40% MPD	7.5	phase separation
	6	0.2M Mg Chloride	0.1M Tris	30% PEG 4000	8.5	dried up
	7		0.1M Cacodylate	1.4M Sodium Acetate	6.5	clear drop
	8	0.2M Sodium Citrate	0.1M Cacodylate	30% isopropanol	6.5	clear drop
	9 _p	0.2M Amm. Acetate	0.1M Sodium Citrate	30% PEG 4000	5.6	phase separation & crystal
	10	0.2M Amm. Acetate	0.1M Acetate	30% PEG 4000	4.6	clear drop
	11		0.1M Citrate	1.0M Amm. Phophate	5.6	clear drop
	12	0.2M Mg Chloride	0.1M Hepes	30% isopropanol	7.5	clear drop
	13	0,2M Sodium Citrate	0.1M Tris	30% PEG 400	8.5	phase separation
	14	0.2M Calcium Chloride	0.1M Hepes	28% PEG 400	7.5	precipitation
	15	0.2M Amm. Sulphate	0.1M Cacodylate	30% PEG 8000	6.5	precipitation
	16°		0.1M Hepes	1.5M Lithium Sulphate	7.5	splinters
	17	0.2M Lithium Sulphate	0.1M Hepes	30% PEG 4000	7.5	phase separation
	18	0.2M Mg Acetate	0.1M Cacodylate	20% PEG 8000	6.5	clear drop
	19	0.2M Amm. Acetate	0.1M Tris	30% isopropanol	8.5	clear drop
	20	0.2M Amm. Sulphate	0.1M Acetate	25% PEG 4000	4.6	heavy precipitatio
	21	0.2M Mg Acetate	0.1M Cacodylate	30% MPD	6.5	fine precipitation
	22	0.2M Sodium Acetate	0.1M Tris	30% PEG 4000	8.5	fine precipitation
	23	0.2M Mg Chloride	0.1M Hepes	30% PEG 400	7.5	skin over drop
	24	0.2M Calcium Chloride	0.1M Acetate	20% isopropanol	4.6	clear drop
	25 ^d		0.1M Imidazole	1.0M Sodium Acetate	7.5	crystal
	26	0.2M Amm. Acetate	0.1M Citrate	30% MPD	5.6	clear drop
	27	0.2M Sodium Citrate	0.1M Hepes	20% isopropanol	7.5	clear drop
	28	0.2M Sodium Acetate	0.1M Cacodylate	30% PEG 8000	6.5	clear drop

	No.	SALT	BUFFER	PRECIPITANT*	рН	RESULT
	29		0.1M Hepes	0.8M Na K Tartrate	7.5	clear drop
	30	0.2M Amm. Sulphate		30% PEG 8000		precipitation
	31	0.2M Amm. Sulphate		30% PEG 4000		precipitation
	32			2.0M Amm. Sulphate		clear drop
5	33		***************************************	4.0M Sodium Formate		precipitation
	34		0.1M Acetate	2.0M Sodium Formate	4.6	precipitation
	35	***************************************	0.1M Hepes	2.0M Na K Phosphate	7.5	precipitation
	36	***************************************	0.1M Tris	8% PEG 8000	8.5	precipitation
	37		0.1M Acetate	8% PEG 4000	4.6	aggregation
10	38	***************************************	0.1M Hepes	1.4M Na Citrate	7.5	heavy precipitation
	39		0.1M Hepes	2.0M Amm. Sulphate 2% PEG 400	7.5	fine precipitation
	40	VIII.	0.1M Citrate	20% PEG 4000, 20% Isopropanol	5.6	fine aggregation
	41		0.1M Hepes	20% PEG 4000, 10% Isopropanol	7.5	clear drop
	42	0.05M K Phosphate		20% PEG 8000		clear drop
15	43			30% PEG 1500		clear drop
	44		•	0.2M Mg Formate		clear drop
	45	0.2M Zn Acetate	0.1M Cacodylate	18% PEG 8000	6.5	heavy precipitation
	46	0.2M Ca Acetate	0.1M Cacodylate	18% PEG 8000	6.5	fine precipitation
	47		0.1M Acetate	2.0M Amm. Sulphate	4.6	heavy precipitation
20	48		0.1M Tris	2.0M Amm. Sulphate	8.5	fine precipitation
	49	1.0M Li Sulphate		2% PEG 8000		med precipitation
	50	1.0M Li Sulphate		15% PEG 8000		heavy precipitation

Final concentration of precipitant used to achieve the result listed.

b. Condition 9 produced two crystals in the single droplet.

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Condition 16 produced a shower of splinters that have arisen from numerous nucleation points within C. the droplet.

d. Condition 25 produced an unusual crystal. Numerous crystalline plates appear to be joined together to form this crystal. X-ray diffraction analysis of this crystal was not successful.

A rapid screening method (generally described in McPherson, 1982, In: Preparation and Analysis of Protein Crystals, 1982, pp. 94-97, John Wiley and Sons, pub.; and J. Crystal Growth , vol. 122, pp. 161-167, 1992) was used. Briefly, hanging drop vapor diffusion experiments were performed using 24-well culture plates. Droplets (about 3 μl) containing about 3 mg/ml of PsFcyRIIa in an equal volume of a mother-liquor were suspended from siliconized coverslips inverted into 24-well tissue culture plates The droplets were equilibrated at about 22°C against well. about 1 ml mother-liquor. Controlled temperature

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incubation was performed in chambers (available from Linbro Inc, distributed by ICN Inc, Costa Mesa CA) at about 22°C. Successful PsFcyRIIa crystallization was performed using the mother-liquor 0.2 M ammonium acetate, 0.1 M citrate pH 5.6 and 30% PEG 4000, at 22°C for between about 3 to about 9 days, or up to 9 months depending upon the purity and concentration of the PsFcyRIIa, resulting in the production of orthorhombic crystals.

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Successful PsFcyRIIa crystallization was also performed using the mother-liquor 0.1 M HEPES pH 7.5 with 1.5 M lithium sulphate, at 22°C for between about 3 to about 9 days, or up to 9 months depending upon the purity and concentration of the PsFcyRIIa, resulting in the production of a series of rod-like splinters of defined structure. The rod-like splinters were analyzed by X-ray diffraction.

B. X-ray Diffraction of Crystalline PsFcyRIIa and Determination of Electron Density Map

The PsFcyRIIa crystals produced as described above in section A were mounted in rayon loops and cryo-cooled to -165°C in mother liquor containing 20% glycerol. heavy atom compounds which sampled a broad range of activities were tested for binding to PsFcyRIIa. (Di-µ-iodo bis[ethylenediamine] di Platinum(II) nitrate) was found to be reactive. Crystals were derivatized by soaking overnight in mother liquor containing about 5 mM Diffraction measurements were made with a M18XHF rotating anode generator (Siemens, Germany) operating at about 40 KV and about 50 mA and using Ni filtered CuKy radiation. The generator was equipped with Franks mirrors (Molecular Structure Corporation, USA), a low-temperature system (Molecular Structure Corporation, USA) and RAXIS IIC and IV image plate detectors (Rigaku, Japan).

The crystals belong to the space group $P2_12_12$ (a = 78.80 Å, b = 100.55 Å, c = 27.85 Å) and diffracted to about 2.4 Å resolution with an R(merge) of 0.065. R(merge) =

 $S(I_i-(IS))/I_i$ summed over all independent reflections where I = intensity. Native and derivative data were collected at 45 minute exposures with an oscillation range of about Diffraction intensities were integrated using DENZO (Otwinowski, et al., Methods in Enzymology, vol. 276, p. 5 307, 1996) and scaled with SCALEPACK (Otwinowski, et al., ibid.). A single heavy atom binding site was located by anomalous difference isomorphous inspection of and In: Protein (Blundell, et al., Patterson maps Crystallography., Horecker, B., Kaplan, N. O., Marmur, J., 10 Scheraga, H. A., Eds., Academic Press, New York, 1976) calculated with the PROTEIN system (Steigeman, Ph.D. Thesis, Technical University, Munich, 1974). parameters were refined and phases were determined in a method of Single Isomorphous Replacement with Anomalous 15 Scattering using the program SHARP (Statistical Heavy-Atom Refinement and Phasing (de La Fortelle, et al., Methods in Enzymology, vol. 276, p. 472, 1996). Merged data in the range of about 18 to about 2.7 Å resolution had an isomorphous R-factor of about 0.162, figure of merit for 20 centric reflections 0.308 and acentric reflections 0.247 and phasing power of 1.127 for centric reflections and 1.081 for acentric reflections (Blundell, ibid.). Phases were modified in a protocol of solvent flattening (Wang, Methods in Enzymology, vol. 115, p. 90, 1985) and histogram 25 mapping (Zhang, et al., Acta Crystallography, vol. A46, p. 377, 1990) in the density modification package DM (Cowtan, ESF-EACBM Newsletter on CCP4 and Crystallography, vol. 31, p. 34, 1994) in the CCP4 suite of programs (Cowtan, ibid.). 2Fo-Fc electron-density maps 30 were displayed using the graphical display program O (Jones et. al., Acta Crystallography, vol. A47, p. 110, 1991). Secondary structural features could be identified at this stage, however the map was difficult to fully interpret and

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trace of the polypeptide. To produce a simplified representation of the electron density, the map was skeletonised (Greer, J. Mol. Biol., vol. 82, p. 279, 1974) using the program BONES (Jones, et al., Coordinates of Killer Inhibitory receptor (Fan, et. al., Nature, vol. 389, p. 96, 1997) and were used as a reference to trace the polypeptide and generate a partial model. calculate subsequent maps density modified phases and phases calculated from the model were combined by the Free-Sim method (Sim, Acta Crystallography, vol. 13, p. 511, 1960).

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Additional data for structure refinement collected at beam line X4A of the National Synchrotron Light Source at Brookhaven National Laboratory (Upton, New York). Using radiation with a wavelength of about 1.058 Å, data were collected on Fuji image plates as exposures of about 100 seconds and oscillation ranges of about 1°. Diffraction images were digitized with a BAS 2000 scanner (Fuji, Japan) and processed as described above, giving an R(merge) of 0.038 for data between about 10 Å and about 1.7 A resolution. Structure refinement was performed with the XPLOR system (Brunger, et al., Science, vol. 235, p. 458, 1987) using protocols including individual temperature energy minimization and slow-cool simulated annealing refinement with bulk solvent correction.

The refined structure of PsFcyRIIa contains all amino acid residues from 1 to 170, together with 33 solvent molecules. The crystallographic residual R-factor and Free R-factor are about 0.253 and about 0.326 respectively for data of from about 7 Å to about 2.0 Å resolution (Brunger, 1987, *ibid.*). Root mean squared deviations from ideality for bond lengths was about 0.01 Å and about 1.45° for angles (Brunger, et al., *Nature*, vol. 355, p. 472, 1992). The resulting data set of the atomic coordinates for PsFcyRIIa is shown in Fig. 4.

C. PsFcyRIIa Structure

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Using the atomic coordinates listed in Table 1, a structure of a dimer of PsFcyRIIa was derived. The structures were computer generated using MOLSCRIPT 2.0 program (available from Avatar Software AB, Heleneborgsgatan 21C, SE-11731 Stockholm, Sweden). The crystal structure reveals PsFcyRIIa in a dimeric form having two 170 amino acid monomers. The two monomers are structurally identical.

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The structure of the PsFcyRIIa residues 1 to 170 consists of two immunoglobulin constant region 2 (C2) type immunoglobulin domains and each domain is comprised of two antiparallel b-sheets, pinned together by a disulfide bond. The first strand of each domain (A strand) is broken in the middle with part forming sheet I (ABE strands) and part forming sheet II (A'GFCC' strands). This structural feature occurs in immunoglobulin variable region (V) type domains and in the natural killer inhibitory receptor (KIR) but not in other C2 domains. The two immunoglobulin-like domains of PsFcyRIIa are quite similar to each other with the rms difference in Ca positions of 1.28 Å for 68 Major differences are in the loops at the residues. N-terminal end of the molecule (BC, C'E and FG loops) and in the position on the C' strand. Some of these loops have been implicated in binding Fc.

The region of association of the two domains in the PsFcyRIIa structure is quite bent, with the angle between the major axes of the domains being approximately 52°. This bend is more severe than other immunoglobulin super family members including 60° for KIR. The domain interface is composed of strands A' from Domain 1 and A & B from Domain 2, where sheet II from each domain forms the interface. Residues whose non-hydrogen atoms lie within 4 Å of the other domain. Water molecules 201, 211, 217-220, 227 and 232 also lie in the interface region.

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Certain structural characteristics indicate that dimer formation between two PsFcyRIIa molecules in the crystal is a preferred interaction. Although the structure of only one PsFcyRIIa molecule (residues 1 to 170) of the crystal has been determined, each PsFcyRIIa molecule comprising the dimer in the crystal is related to the other PsFcyRIIa molecule in the crystal by a 2-fold crystallographic axis. By applying the transformation:

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$$(-1 \ 0 \ 0) \ (x) \ (0.)$$
 $(0 \ -1 \ 0) \ (y) + (100.55)$
 $(0 \ 0 \ 1) \ (z) \ (0.)$

to the coordinates given in Table 1 a dimer is formed (Fig. 4), with the interface composed of sheet II from each PsFcyRIIa molecule. The coordinates of the FcyRIIa dimer are represented in Table 2. The contact area is $(\sim 400 \text{ Å}^2)$ and this interface has more substantial hydrophobic character than the Domain 1-Domain 2 interface. Residues whose non-hydrogen atoms lie within 4 Å of the other molecule or water molecule 207 on the axis are 119, 121, 124-126, 150, 152 and 158-161, with residues 148, 163 and 164 also making a close approach. This type of domain interaction is not novel for immunoglobulins because V regions of antibodies pair in a similar manner. This type of interaction, however, has not been observed for C2 domains. Due to the size and character of this contact it suggests that this hitherto unforeseen interaction has physiological relevance.

Additional structural considerations support this conclusion. The crystal structure described above suggests that, if an FcyRIIa molecule is oriented with the C-terminus toward a cell membrane containing the receptor, then the putative Fc binding region of the receptor does not point away from the cell but to one side. Thus, forming a dimer between two FcyRIIa molecules in a cell membrane, the two potential Fc binding regions are brought

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near each other and point away from the cell because the dimer axis points away from the cell. This orientation positions the potential Fc binding sites ideally for interaction with ligand (i.e., IgG), enabling the ligand binding site to be composed of regions from two receptor molecules. Involving two receptor molecules in a binding event has implications for cellular signal transduction because dimerization of the extracellular domains would bring the cytoplasmic domains of the two receptors together to initiate a cellular signal transduction response.

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Fig. 4 shows a graphical representation of the dimer of PFcvRIIa. Two Ig-like domains (Domains 1 and 2) are shown in each monomer of each dimer. The first amino acid residue of the amino (NH2) terminus of the protein is indicated by residue number 0. The last amino acid residue of the carboxyl (COOH) terminus of the protein is indicated by residue 170. Numbering of amino acid residues from the NH2 terminus to the COOH terminus are shown where possible. Certain residues were omitted for clarity. illustrates the amino acid residues that comprise each beta sheet of Domain 1 and Domain 2 of PFcyRIIa. In Domain 1, strand A includes residues 5-10, strand A' residues 14-17, strand B includes residues 20-28, strand C includes residues 37-41, strand C' includes residues 44-46, strand E includes residues 52-58, strand F includes residues 63-70 and strand G includes residues 78-84. Domain 2, strand A includes residues 87-92, strand A' includes residues 95-97, strand B includes residues 102-110, strand C includes residues 117-122, strand C' includes residues 125-131, strand E includes residues 134-139, strand F includes residues 146-155, strand G includes residues 158-162 and strand G' includes residues 163-169. Fig. 6 shows the stereo view of the structure of the polypeptide shown in Fig. 4 in stereo.

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A graphical representation of the three dimensional structure shown in Fig. 4 was used to determine the location of amino acid residues involved in the binding of FcyRIIa to IgG. Fig. 7 shows the location of the mutated alanine residues (indicated by the black balls) involved in the loss of binding of FcyRIIa to IgG. The residues shown in Fig. 7 were identified using recombinant mutants of FcyRIIa, in which residues were replaced with alanine and were found to disrupt or decrease IgG binding to FcyRIIa (described in Hulett, et al., 1994, ibid.; Hulett, et al., 1995, ibid.). Fig. 8 shows an expanded view of the IgG binding region showing position and side chains of amino acids involved in IgG binding to FcyRIIa, as shown by production of nucleic acid molecules having mutations in this region that encode an FcyRIIa protein having reduced binding to IgG.

Fig. 9 shows an expanded view of the IgG binding region and the amino acid residues, which when mutated to alanine, improve IgG binding.

The interface between the two dimers illustrated in the graphical representation of the three dimensional structure shown in Fig. 4 was further analyzed. shows an expanded view of the region of one FcyRIIa monomer that contributes to the dimer interface. In Fig. 10, the region has been rotated about 90° in x, where x is The y carbon of amino acid horizontal to the page. residues contributing to the interface are shown as black balls and are numbered according to the residue numbering of SEQ ID NO:3.

Example 7 30

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This example describes analysis of N-terminal sequence of PsFcyRIIa protein by electrospray ionization mass spectrometry.

To determine the N-terminal amino acid sequence of PsFcyRIIa protein, the heterogeneity of the N-linked

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glycosylation mass spectrometry was carried out as follows. Various samples were prepared by combining about 1 to about 100 picomolar (pmol) of PsFcyRIIa protein in about 2 μ l to about 4 μ l of 50% CH₃CN containing 0.1% acetic acid. samples were infused at a flow rate of about 0.2 μ l/min into a Perkin Elmer Sciex API-300 triple quadrupole mass spectrometer fitted with a micro-ionspray ion source and The mass scale was operated in the Q1 scan mode. calibrated at eight points over the 3000 u mass range, to an accuracy equivalent to ± 0.01%, using singly charged Mass spectra (typically poly(propylene glycol) ions. 30-100 scans) were recorded over the mass rand m/z200 u to 3000 u with a constant peak width of 0.6 u (peak width at half-height), and were processed by signal-averaging, manual mass determination and transformation using PE-Sciex The results indicated that two Biomultiview software. major species of protein having different N-terminal sequence were present in the solution of purified PsFcyRIIa One species had a N-terminal sequence comprising SEQ ID NO:4 and the other species had a N-terminal sequence with an additional Ala at the 5' end of the protein (e.g., Ala-Ala-Pro-).

Example 8

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This example describes the modeling of the three dimensional structure of the Fce receptor I (FceRI) in both monomeric and dimeric forms.

The extracellular regions of the human Fc epsilon receptor type I (FceRI) and the human Fc gamma Receptor type II a (Fc\(\gamma\)RIIa) show a sequence identity of about 38\(\gamma\) (for 172 residues). The final sequence alignment used in this modeling work is shown in Fig. 13. The X-ray crystallographic structure of the human Fc\(\gamma\)RIIa was determined by the present inventors (Table 1). The 3-dimensional coordinates of Fc\(\gamma\)RIIa in Table 1 differ from those used as the template to build a 3-dimensional model

of the human FceRI by orientation of the imidazole ring of His 108 and one round of refinement.

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Secondary structure prediction performed on FceRI confirmed the validity of the alignment given in Fig. 13 and showed the pattern of β strands is the same in both FceRI and FcyRIIa. The secondary structure prediction methods used were PHD (B. Rost et al., CABIOS, vol. 10, 266-275(1994)) and PREDATOR (D. Frishman and P. Argos, Proteins, vol. 27, 329-335(1997)).

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MODELER (A. Sali and T.L. Blundell, J. Mol. Biol., vol. 779-815(1993)) as implemented in InsightII_Homology software package (Insight II (97.0), MSI, San Diego) was used to generate 3-dimensional models of FceRI using a number of different initial sequence alignments and two structural templates of FcyRIIa. One of the structural templates was the 3-dimensional coordinates of FcyRIIa where, for the residues that had alternative side-chain conformations (residue numbers 10, 21, 33, 57, 60, 61, 65, and 89), the conformations labeled 'A' were selected while in the other template the conformations labeled 'B' were selected. In each Modeler run 5 structural models of FceRI were generated. The following parameter values or options were used: 'library_schedule' of 1, 'max_var_iterations' of 300, 'md level' of 'refinel', 'repeat_optimization' of 3, and 'max_molpdf' of 1e6. The best model from these runs had the sequence alignment given in Fig. 13, and used the structural template of FcyRIIa, where residues 10, 21, 33, 57, 60, 61, 65, and 89 had side-chains in the 'A' conformation. The criteria for judging the 'best' model included the lowest value of the Modeler objective function (or -1.0xln (Molecular probability density function=Mpdf)), 'well-behaved' PROSAII (M. Sippl, Proteins, vol. 17, 355-362(1993)) residue energy plot for the model (for example, negative residue energy scores throughout the sequence), and 'well-behaved'

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et al., Science, vol. PROFILES-3D (J.U. Bowie

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164-170(1991)) local 3D-1D compatibility score plot (for example, positive plot scores throughout the sequence).

Next, Modeler was used to generate 20 different structural models of FceRI using the sequence alignment and template selected above, and using the parameter values and options listed above. The model with the lowest -ln(Mpdf) value (i.e. 957.2) was then selected as the template to generate structural models of the FceRI sequence in the At the end of four such next cycle of Modeler runs. cycles, the 'best' 3-dimensional model of the FceRI structure had a -ln(Mpdf) value of 643.2. selected as the final structural model of the FceRI monomer, and the corresponding heavy (non-hydrogen) atom cartesian coordinates are represented in Table 3. A 'worm' representation of the structure is shown in Fig. 14. structure was validated with the programs PROSAII, and PROCHECK (R.M.Laskowski et al., PROFILES-3D, J.Appl.Cryst. vol. 26, 283-291(1993)).

Finally, the same coordinate transformation that generates a dimer from the FcyRIIa monomer was applied to the above model of the FceRI monomer. The interface of the resultant dimer was optimized by selecting alternative rotamers for the Glu 161 and Tyr 150 residues with the Auto_Rotamer option of the InsightII_Homology module (MSI, San Diego), and then adding hydrogen atoms to the dimer model and energy minimizing it keeping all heavy atoms fixed, except for Tyr 150 and Glu 161 where only the The program Discover v. backbone atoms were kept fixed. 2.98 (MSI, San Diego) was used for the energy minimization with the CFF91 force field and a distance-dependent dielectric constant of 1.0 \times r, and the minimization was done with the conjugate gradients' method until the maximum energy gradient was less than 0.10 kcal/Å. The cartesian coordinates of the resultant model of the FceRI dimer are

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represented in Table 4 and a 'worm' representation of the dimer model is shown in Fig. 15. This model of the FceRI dimer has a shape complementarity or Sc value(see M.C. Lawrence and P.M. Colman, J. Mol. Biol., vol. 234, 946-950(1993)) at the monomer-monomer interface of 0.64 and an electrostatic complementarity value - for the fully solvated case, using the Spearman correlation coefficient - (see A. J. McCoy, V.C. Epa, and P.M. Colman, J. Mol. Biol.. vol. 268, 570-584(1997)) or ECSFS at the monomer-monomer interface of 0.08. These compare with 0.80 and 0.32, respectively, for the FcyRIIa dimer. reduced complementarity values for the FcgRI dimer compared to the FcyRIIa dimer indicates that formation of the FceRI dimer, as built herein, is energetically less favored than it is in the FcyRIIa case. However, we note that the interaction with the β or γ chains of the FceRI has not been taken into consideration. Fig. 16 shows a molecular surface representation of the FceRI dimer model.

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The model of the 3-dimensional structure of FceRI monomer represented by the coordinates in Table 3 or the FceRI dimer represented by the coordinates in Table 4 may be used as a basis for drug design in the same manner as that described for the crystallographic coordinates of FcyRIIa herein.

25 Example 9

The following example demonstrates the crystallization of the Fce receptor I (FceRI).

Recombinant molecule pFceRI, containing a nucleic acid molecule encoding a soluble form of human FceRI (sFceRI) operatively linked to baculovirus polyhedron transcription control sequences was produced as described for the pFcyRIIa molecule in Examples 1-3. Briefly, the recombinant soluble FceRI was generated by placing a translation termination codon at the position 173 which normally encodes a Pro in the sequence Ile, Lys, Ala, Pro,

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at the C-terminal end of the second domain as set forth in the sequence represented in Fig. 13. Soluble FceRI was expressed in baculovirus expression system 'Bac to Bac' supplied by GIBCO. Infections of SF21 or Sf9 cells were performed as described by the manufacturer. Briefly, the recombinant FcyRIIa molecule was ligated into pVL1392 baculovirus shuttle plasmid (available from Pharmingen, San Diego, CA) to produce a recombinant molecule referred to herein as pVL-sFceRI. The recombinant molecule pVL-sFceRI was subsequently co-transfected with baculovirus strain (available from Pharmingen) into Spodoptera frugiperda 21 (Sf-21) cells (available from Invitrogen Corp., San Diego, CA) to produce S. frugiperda:pVL-sFceRI cells. 65-70 hours following infection, supernatants were harvested and soluble receptor was purified by affinity chromatography on an anti-FceRI antibody (3B4) monoclonal antibody-sepharose 4B affinity column, similar to the processes described for FcyRIIa in Example 5. The column was washed with 10 mM Tris pH 7.5 and eluted with 0.1 ${\rm M}$ sodium acetate, 0.5M sodium chloride, pH4.0. The purified protein was concentrated and used in crystallization trials as described above for FcyRIIa (Example 6). Crystals were produced under several conditions as follows:

- (a) 0.2M calcium acetate; 0.1M sodium cacodylate, pH6.5; 18% w/v polyethylene glycol (PEG) 8000;
- (b) 0.1M sodium cacodylate, pH6.0 or pH5.5; 10% v/v 2-propanol; 20% w/v PEG 4000;
- (c) 0.2M tri sodium citrate dihydrate; 0.1M sodium cacodylate pH6.5; 30% v/v 2-propanol.

The structure of the FceRI crystals obtained by these experiments can be used in X-ray diffraction analysis and/or in molecular replacement and modeling strategies as described herein.

Example 10

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This example describes the modeling of the three dimensional structure of the Fc γ receptor III (Fc γ RIIIb) in monomeric form.

The extracellular regions of the human Fc gamma receptor type III (FcyRIIIb) and the human Fc gamma Receptor type II a (FcyRIIa) show a sequence identity of about 53% (for 174 residues). The final sequence alignment used in this modeling work is shown in Fig. 18. The X-ray crystallographic structure of the human FcyRIIa was determined by the present inventors (Table 1) as described in Examples 1-7. The 3-dimensional coordinates of FcyRIIa in Table 1 differ from those used as the template to build a 3-dimensional model of the human FcyRIIIb by orientation of the imidazole ring of His 108 and one round of refinement.

MODELER (A. Sali and T.L. Blundell, J. Mol. Biol., implemented as in 779-815(1993)) vol. InsightII_Homology software package (Insight II (97.0), MSI, San Diego) was used to generate 3-dimensional models of FcyRIIIb using a number of different initial sequence alignments and two structural templates of FcyRIIa. structural template that was used was the 3-dimensional coordinates of FcyRIIa where, for the residues that had alternative side-chain conformations (residue numbers 10, 21, 33, 57, 60, 61, 65, and 89), the conformations labeled 'A' were selected. In each Modeler run 5 structural models of FcyRIIIb were generated. The following parameter values 'library schedule' used: options were or 'max_var_iterations' of 300, 'md_level' of 'refinel', 'repeat_optimization' of 3, and 'max_molpdf' of 1e6. best model from these runs had the sequence alignment given in Fig. 18, and used the structural template of FcyRIIa, where residues 10, 21, 33, 57, 60, 61, 65, and 89 had side-chains in the 'A' conformation. The criteria for

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judging the 'best' model included the lowest value of the Modeler objective function (or -1.0xln (Molecular probability density function=Mpdf)), 'well-behaved' PROSAII (M. Sippl, Proteins, vol. 17, 355-362(1993)) residue energy plot for the model (for example, negative residue energy scores throughout the sequence), and 'well-behaved' PROFILES-3D (J.U. Bowie et al., Science, vol. 164-170(1991)) local 3D-1D compatibility score plot (for example, positive plot scores throughout the sequence).

Next, Modeler was used to generate 20 different structural models of FcyRIIIb using the sequence alignment and template selected above, and using the parameter values and options listed above. The model with the lowest -ln(Mpdf) value (i.e. 933.3) was then selected as the final structural model of the FcyRIIIb monomer, and the corresponding heavy (non-hydrogen) atom cartesian coordinates are represented in Table 5. This structure was validated with the programs PROSAII, PROFILES-3D, and PROCHECK (R.M. Laskowski et al., J.Appl.Cryst. vol. 26, 283-291(1993)).

The model of the 3-dimensional structure of FcyRIIIb monomer represented by the coordinates in Table 5 may be used as a basis for drug design in the same manner as that described for the crystallographic coordinates of FcyRIIa herein.

While various embodiments of the present invention have been described in detail, it is apparent that modifications and adaptations of those embodiments will occur to those skilled in the art. It is to be expressly understood, however, that such modifications and adaptations are within the scope of the present invention, as set forth in the following claims.

What is claimed is:

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1. A model of an Fc receptor (FcR) protein, wherein said model represents a three dimensional structure that substantially conforms to the atomic coordinates of Table 1.

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- 2. The model of Claim 1, wherein said structure substantially conforms to the atomic coordinates and B-values represented by Table 1.
- 3. The model of Claim 1, wherein said structure is monomeric.
 - 4. The model of Claim 1, wherein said structure is dimeric.
 - 5. The model of Claim 1, wherein said structure substantially conforms to the atomic coordinates of a table selected from the group consisting of Table 2, Table 3, Table 4 and Table 5.
 - 6. The model of Claim 1, wherein at least about 50% of said structure has an average root-mean-square deviation (RMSD) of less than about 1.5\AA for backbone atoms in secondary structure elements in each domain of said structure.
 - 7. The model of Claim 1, wherein at least about 50% of common amino acid side chains between said structure and a structure comprising said atomic coordinates have an average root-mean-square deviation (RMSD) of less than about 1.5Å.
 - 8. The model of Claim 1, wherein said FcR protein comprises an amino acid sequence that is at least about 25% identical to an amino acid sequence selected from the group consisting of SEQ ID NO:3, SEQ ID NO:10, SEQ ID NO:11 and SEQ ID NO:12.
 - 9. The model of Claim 1, wherein said FcR protein comprises an amino acid sequence that is at least about 40% identical to an amino acid sequence selected from the group

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consisting of SEQ ID NO:3, SEQ ID NO:10, SEQ ID NO:11 and SEQ ID NO:12.

- 10. The model of Claim 1, wherein said FcR protein comprises an amino acid sequence that is at least about 60% identical to an amino acid sequence selected from the group consisting of SEQ ID NO:3, SEQ ID NO:10, SEQ ID NO:11 and SEQ ID NO:12.
- 11. The model of Claim 1, wherein said FcR protein comprises an amino acid sequence selected from the group consisting of: SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, SEQ ID NO:13, a mutant of any of said amino acid sequences, and an allelic variant of any of said amino acid sequences.
- 12. The model of Claim 1, wherein said FCR protein comprises an amino acid sequence selected from the group consisting of: an amino acid sequence selected from the group consisting of SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12, SEQ ID NO:13; a mutant of SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12 or SEQ ID NO:13; and an allelic variant of SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11, SEQ ID NO:12 or SEQ ID NO:13.
 - 13. The model of Claim 1, wherein said FcR protein is selected from the group consisting of Fc γ RI protein, Fc γ RIIa protein, Fc γ RIIb protein, Fc γ RIIc protein, Fc γ RIII protein, Fc α RI protein and structural homologues of any of said FcR proteins.
 - 14. The model of Claim 1, wherein said FcR protein is selected from the group consisting of FcγRI protein, FcγRIIa protein, FcγRIIa protein, FcγRIII protein, FcγRIII protein, FcαRI protein and FcαRI protein.

15. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FcyRIIa protein monomer, an FcyRIIa protein dimer and structural homologues of said FcyRIIa proteins.

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16. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FceRI protein dimer, an FceRI protein monomer and structural homologues of said FceRI proteins.

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- 17. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FcyRI protein dimer, an FcyRI protein monomer and structural homologues of said FcyRI protein.
- 18. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FcyRIIb protein dimer, an FcyRIIb protein monomer and structural homologues of said FcyRIIb protein.
- 19. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FcyRIIc protein dimer, an FcyRIIc protein monomer and structural homologues of said FcyRIIc protein.
- 20. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an FcyRIIIb protein dimer, an FcyRIIIb protein monomer and structural homologues of said FcyRIIIb protein.
- 21. The model of Claim 1, wherein said FcR protein is selected from the group consisting of an Fc α RI protein dimer, an Fc α RI protein monomer and structural homologues of said Fc α RI protein.
 - 22. The model of Claim 1, wherein said atomic coordinates are generated by the method comprising:
 - (a) providing an Fc γ RIIa protein in crystalline form;
 - (b) generating an electron-density map of said crystalline FcyRIIa protein; and

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(c) analyzing said electron-density map to produce said atomic coordinates.

- 23. The model of Claim 22, wherein said crystalline FcyRIIa protein is produced by a method comprising: combining FcyRIIa protein with a mother liquor buffer selected from the group consisting of an acetate salt buffer and a sulphate buffer, and inducing crystal formation to produce said crystalline FcyRIIa protein.
- 24. The model of Claim 23, wherein said acetate buffer comprises about 200 mM ammonium acetate, about 100 mM sodium citrate and about 30% PEG 4000, said buffer having a pH of about 5.6.
- 25. The model of Claim 23, wherein said sulphate buffer comprises about 0.1 M HEPES and about 1.5 M lithium sulphate, said buffer having a pH of about 7.5.
- 26. The model of Claim 22, wherein said step of generating an electron-density map comprises analyzing said crystalline FcyRIIa protein by X-ray diffraction.
- 27. The model of Claim 22, wherein said crystalline Fc γ RIIa protein is derivatized in Di- γ -iodo bis{ethylenediamine} di Platinum(II) nitrate prior to said X-ray diffraction.
- 28. The model of Claim 22, wherein said crystalline Fc γ RIIa protein is derivatized in about 5 mM Di- γ -iodo bis[ethylenediamine] di Platinum(II) nitrate prior to said X-ray diffraction.
- 29. The model of Claim 1, wherein said model is a computer image generated by a computer-readable medium encoded with a set of three dimensional coordinates of said three dimensional structure, wherein, using a graphical display software program, said three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

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30. A computer-assisted method of structure based drug design of bioactive compounds, comprising:

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providing a model of an Fc receptor (FcR) protein, wherein said model represents a three dimensional structure that substantially conforms to the atomic coordinates of Table 1;

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- designing a chemical compound using said model; and,
 - c. chemically synthesizing said chemical compound.
- The method of Claim 30, wherein said method 31. further comprises:
- evaluating the bioactivity of said synthesized chemical compound.
- 32. The method of Claim 30, wherein said three dimensional structure comprises the atomic coordinates listed in Table 1.
 - The method of Claim 30, wherein said three dimensional structure is dimeric.
 - The method of Claim 30, wherein said three dimensional structure comprises the atomic coordinates listed in a table selected from the group consisting of Table 2, Table 3, Table 4, and Table 5.
 - The method of Claim 30, wherein said model comprises a computer image generated when the atomic coordinates listed in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of said image and visualizing said electronic file on a computer capable of representing said electronic file as a three dimensional image.
- 30 The method of Claim 30, wherein said step of designing comprises computational screening of one or more databases of chemical compounds in which the three dimensional structure of said compounds are known.

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- 37. The method of Claim 36, further comprising interacting a compound identified by said screening step with said model by computer.
- 38. The method of Claim 30, wherein said step of designing comprises directed drug design.

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- 39. The method of Claim 30, wherein said step of designing comprises random drug design.
- 40. The method of Claim 30, wherein said step of designing comprises grid-based drug design.
- 41. The method of Claim 30, wherein said step of designing comprises selecting compounds which are predicted to mimic said three dimensional structure of said FcR protein.
- 42. The method of Claim 30, wherein said step of designing comprises selecting compounds which are predicted to bind to said three dimensional structure of said FcR protein.
- 43. The method of Claim 30, wherein said bioactivity is selected from the group consisting of inhibiting binding of said FcR protein to an immunoglobulin protein, binding to said FcR protein, binding to an immunoglobulin which is capable of binding to said FcR protein, inhibiting phagocytosis of said immunoglobulin protein, inhibiting dimerization of said FcR protein, stimulating cellular signal transduction though said FcR protein, and stimulating release of cytokines through said FcR protein.
- 44. The method of Claim 30, wherein said FcR protein is FcyRIIa and said bioactivity is selected from the group consisting of inhibiting binding of FcyRIIa protein to IgG, inhibiting phagocytosis of IgG, inhibiting dimerzation of FcyRIIa protein, stimulating cellular signal transduction though an FcyRIIa protein, stimulating release of cytokines selected from the group consisting of IL-6 and IL-12.
- 45. The method of Claim 30, wherein said FcR protein is FcyRIIIb and said bioactivity is selected from the group

consisting of inhibiting binding of FcyRIIIb protein to IgG, inhibiting phagocytosis of IgG, inhibiting dimerzation of FcvRIIIb protein, stimulating cellular transduction though an FcyRIIIb protein, stimulating release of cytokines selected from the group consisting of IL-6 and IL-12.

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- 46. The method of Claim 30, wherein said FcR protein is FceRI and said bioactivity is selected from the group consisting of inhibiting binding of FceRI protein to IqE, inhibiting phagocytosis of IqE, inhibiting dimerzation of FccRI protein, stimulating cellular signal transduction though an FccRI protein, stimulating release of histamine and serotonin by mast cells and inhibiting release of histamine and serotonin by mast cells.
- 47. A computer-assisted method of structure based drug design of bioactive compounds, comprising:
- providing a model of an Fc receptor (FcR) protein, wherein said model represents a three dimensional structure that substantially conforms to the coordinates selected from the group consisting of atomic coordinates represented by Table 1; atomic coordinates represented by Table 2; atomic coordinates represented by Table 3; atomic coordinates represented by Table 4; and atomic coordinates represented by Table 5;
- 25 designing a chemical compound using said model; and,
 - chemically synthesizing said chemical compound. c.
 - A computer-assisted method of structure based drug design of bioactive compounds, comprising:
 - providing a model of a three dimensional structure of an Fc receptor (FcR) protein selected from the group consisting of FcyRIIa, FcyRIIIb and FceRI;
 - b. designing a chemical compound using said model; and,
- 35 chemically synthesizing said chemical compound. c.

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49. A three dimensional computer image of the three dimensional structure of an FcR protein.

- 50. The image of Claim 49, wherein said structure substantially conforms with the three dimensional coordinates selected from the group consisting of the three dimensional coordinates listed in Table 1; the three dimensional coordinates listed in Table 2; the three dimensional coordinates listed in Table 3; the three dimensional coordinates listed in Table 4; and the three dimensional coordinates listed in Table 5.
- 51. The image of Claim 49, wherein said computer image is generated when a set of three dimensional coordinates comprising said three dimensional coordinates are analyzed on a computer using a graphical display software program to create an electronic file of said image and visualizing said electronic file on a computer capable of representing electronic file as a three dimensional image.
- 52. The image of Claim 49, wherein said three dimensional computer image is represented by a two dimensional image selected from the group consisting of Fig. 4, Fig. 6, Fig. 7, Fig. 8, Fig. 9, Fig. 10, Fig. 14, Fig. 15 and Fig. 16.
 - 53. The image of Claim 49, wherein said three dimensional computer image is used to design a therapeutic compound.
 - 54. A computer-readable medium encoded with a set of three dimensional coordinates of an FcR protein having a three dimensional structure that substantially conforms to the atomic coordinates of Table 1, wherein, using a graphical display software program, said three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

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55. A computer-readable medium encoded with a set of three dimensional coordinates selected from the group consisting of the three dimensional coordinates represented in Table 1, the three dimensional coordinates represented in Table 2, the three dimensional coordinates represented in Table 3, the three dimensional coordinates represented in Table 4, and the three dimensional coordinates represented in Table 5, wherein, using a graphical display software program, said three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

- 56. A model of the three dimensional structure of an FcR protein selected from the group consisting of Fc γ RI protein, Fc γ RIIb protein, Fc γ RIIc protein, Fc γ RIIIb protein, Fc α RI protein and Fc α RI protein, said model being produced by the method comprising:
- (a) providing an amino acid sequence of an FcyRIIa protein and an amino acid sequence of said FcR protein;
- (b) identifying structurally conserved regions shared between said FcγRIIa amino acid sequence and said FcR protein amino acid sequence; and
- (c) determining atomic coordinates for said FcR protein by assigning said structurally conserved regions of said FcR protein to a three dimensional structure using a three dimensional structure of said FcyRIIa protein which substantially conforms to the atomic coordinates represented in Table 1, to derive a model of said three dimensional structure of said FcR protein amino acid sequence.
- 57. The model of Claim 56, wherein said FcyRI protein amino acid sequence comprises SEQ ID NO:7; wherein said FcyRIIb protein amino acid sequence comprises SEQ ID NO:5; wherein said FcyRIIc protein amino acid sequence comprises

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SEQ ID NO:6; wherein said FcyRIIIb protein amino acid sequence comprises SEQ ID NO:8; wherein said FceRI protein amino acid sequence comprises SEQ ID NO:9; and wherein said FcαRI protein amino acid sequence comprises SEO ID NO:13.

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58. A therapeutic composition that, when administered to an animal, reduces IqG-mediated tissue damage, said therapeutic composition comprising an inhibitory compound that inhibits the activity of an Fcy receptor (FcyR) protein, said inhibitory compound being identified by the method comprising:

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- providing a three dimensional structure of an FcyR protein selected from the group consisting of FcyRI, FcyRIIa, FcyRIIb, FcyRIIc and FcyRIIIb, wherein said dimensional structure of said FcyR substantially conforms to atomic coordinates represented by Table 1:
- (b) using said three dimensional structure of said FcYR protein to design a chemical compound selected from the group consisting of a compound that inhibits binding of FcyR protein to IqG, a compound that substantially mimics the three dimensional structure of FcyR protein and a compound that inhibits binding of FcyR protein with a molecule that stimulates cellular signal transduction through an FcyR protein;
- (c) chemically synthesizing said compound; and
- evaluating the ability of said synthesized chemical compound to reduce IgG-mediated tissue damage.
- The composition of Claim 58, wherein said IgG-mediated tissue damage results from a biological response selected from the group consisting of IgG-mediated hypersensitivity, IgG-mediated recruitment of inflammatory cells, and IgG-mediated release of inflammatory modulators.

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60. The composition of Claim 58, wherein said structure substantially conforms with the atomic coordinates represented in Table 1.

61. The composition of Claim 58, wherein said chemical compound is selected from the group consisting of an inorganic compound and an organic compound.

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- 62. The composition of Claim 58, wherein said chemical compound is selected from the group consisting of oligonucleotides, peptides, peptidomimetic compounds and small organic molecules.
- 63. The composition of Claim 58, wherein said chemical compound is selected from the group consisting of an analog of said FcyR protein, a substrate analog of said FcyR protein and a peptidomimetic compound of said FcyR protein.
- 64. The composition of Claim 58, wherein said composition further comprises a component selected from the group consisting of an excipient, an adjuvant, and a carrier.
- 65. A therapeutic composition that, when administered to an animal, enhances IgG-mediated responses, said therapeutic composition comprising a stimulatory compound that stimulates the activity of an Fcγ receptor (FcγR) protein, said stimulatory compound being identified by the method comprising:
 - (a) providing a three dimensional structure of an FcγR protein selected from the group consisting of FcγRI, FcγRIIa, FcγRIIb, FcγRIIc and FcγRIIIb, wherein said three dimensional structure of said FcγR protein substantially conforms to atomic coordinates represented by Table 1;
 - (b) using said three dimensional structure of said $Fc\gamma R$ protein to design a chemical compound selected from the group consisting of a compound that stimulates binding of $Fc\gamma R$ protein to IgG, a compound that

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substantially mimics the three dimensional structure of Fc γ R protein and a compound that stimulates binding of Fc γ R protein with a molecule that stimulates cellular signal transduction through an Fc γ R protein;

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- (c) chemically synthesizing said chemical compound; and
- (d) evaluating the ability of said synthesized chemical compound to enhance IgG-mediated responses.
- 66. A therapeutic composition that, when administered to an animal, reduces IgE-mediated responses, said therapeutic composition comprising an inhibitory compound that inhibits the activity of an Fce receptor I (FceRI) protein, said inhibitory compound being identified by the method comprising:
- (a) providing a three dimensional structure of an FceRI protein, wherein said three dimensional structure of said FceRI protein substantially conforms to the atomic coordinates selected from the group consisting of the atomic coordinates represented by Table 1, the atomic coordinates represented by Table 2, the atomic coordinates represented by Table 3, the atomic coordinates represented by Table 4 and the atomic coordinates represented by Table 5;
 - (b) using said three dimensional structure of said FceRI protein to design a chemical compound selected from the group consisting of a compound that inhibits binding of FceRI protein to IgE, a compound that substantially mimics the three dimensional structure of FceRI protein and a compound that inhibits binding of FceRI protein with a molecule that stimulates cellular signal transduction through an FceRI protein;
 - (c) chemically synthesizing said chemical compound; and
- (d) evaluating the ability of said synthesized chemical compound to reduce IgE-mediated responses.

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67. The composition of Claim 66, wherein said IgE-mediated response results from a biological response selected from the group consisting of IgE-mediated hypersensitivity, IgE-mediated recruitment of inflammatory cells, and IgE-mediated release of inflammatory modulators.

- 68. The composition of Claim 66, wherein said structure comprises the atomic coordinates represented in Table 3.
- 69. The composition of Claim 66, wherein said structure comprises the atomic coordinates represented in Table 4.
- 70. The composition of Claim 66, wherein said chemical compound is selected from the group consisting of an inorganic compound and an organic compound.
- 71. The composition of Claim 66, wherein said chemical compound is selected from the group consisting of oligonucleotides, peptides, peptidomimetic compounds and small organic molecules.
 - 72. The composition of Claim 66, wherein said chemical compound is selected from the group consisting of an analog of said FceR protein, a substrate analog of said FceRI protein and a peptidomimetic compound of said FceRI protein.
 - 73. The composition of Claim 66, wherein said composition further comprises a component selected from the group consisting of an excipient, an adjuvant, and a carrier.
 - 74. A therapeutic composition that, when administered to an animal, enhances IgE-mediated responses, said therapeutic composition comprising a stimulatory compound that stimulates the activity of an Fce receptor I (FceRI) protein, said stimulatory compound being identified by the method comprising:
- (a) providing a three dimensional structure of an FceRI protein, wherein said three dimensional structure

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of said FCERI protein substantially conforms to the atomic coordinates selected from the group consisting of the atomic coordinates represented by Table 1, the atomic coordinates represented by Table 2, the atomic coordinates represented by Table 3, the atomic coordinates represented by Table 4 and the atomic coordinates represented by Table 5;

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- (b) using said three dimensional structure of said FceRI protein to design a chemical compound selected from the group consisting of a compound that stimulates binding of FceRI protein to IgE, a compound that substantially mimics the three dimensional structure of FceRI protein and a compound that stimulates binding of FceRI protein with a molecule that stimulates cellular signal transduction through an FceRI protein;
- (c) chemically synthesizing said chemical compound; and
- (d) evaluating the ability of said synthesized chemical compound to enhance IgE-mediated responses.
- 75. A method to determine a three dimensional structure of an FcR protein, said method comprising
- (a) providing an amino acid sequence of an FCR protein selected from the group consisting of FCYRI protein, FCYRIIb protein, FCYRIIc protein, FCYRIIIb protein, FCCRI protein and FCCRI protein, wherein the three dimensional structure of said FCR protein is not known;
- (b) analyzing the pattern of folding of said amino acid sequence in a three dimensional conformation by fold recognition; and
- 30 (c) comparing said pattern of folding of said FcR protein amino acid sequence with the three dimensional structure of FcyRIIa protein to determine the three dimensional structure of said FcR protein, wherein said three dimensional structure of said FcyRIIa protein

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substantially conforms to the atomic coordinates represented in Table 1.

- 76. A method to derive a model of the three dimensional structure of an FcR protein, said method comprising the steps of:
- (a) providing an amino acid sequence of an $Fc\gamma RIIa$ protein and an amino acid sequence of an FcR protein;
- (b) identifying structurally conserved regions shared between said FcyRIIa amino acid sequence and said FcR protein amino acid sequence;
- (c) determining atomic coordinates for said target structure by assigning said structurally conserved regions of said FcR protein to a three dimensional structure using a three dimensional structure of an FcyRIIa protein based on atomic coordinates that substantially conform to the atomic coordinates represented in Table 1 to derive a model of the three dimensional structure of said FcR protein amino acid sequence.
- 77. The method of Claim 76, further comprising assigning atomic coordinates for side chains of said FcR protein by determining sterically allowable positions using a library of rotamers.
 - 78. A method to derive a three dimensional structure of a crystallized FcR protein, said method comprising the steps of:
 - (a) comparing the Patterson function of a crystallized FcR protein with the Patterson function of crystalline Fc γ RIIa protein to produce an electron-density map of said crystallized FcR protein; and
 - (b) analyzing said electron-density map to produce said three dimensional structure of said crystallized FCR protein.
- 79. The method of Claim 78, further comprising the step of electronically simulating said three dimensional

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structure of said crystallized FcR protein to derive a computer image of said three dimensional structure of said crystallized FcR protein.

80. The method of Claim 78, further comprising the step of rotating said Patterson function of said crystallized FcR protein on said Patterson function of said crystalline FcyRIIa protein to determine the correct orientation of said crystallized FcR protein in a crystal of said crystallized FcR protein to identify the initial phases of said crystallized FcR protein.

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81. A composition comprising Fc γ RIIa protein in a crystalline form.

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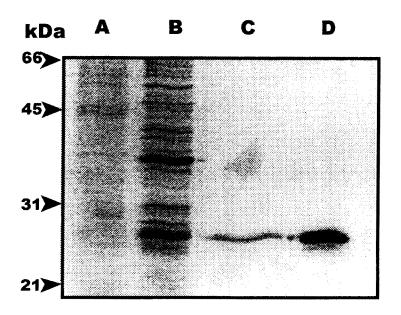


FIG. 1

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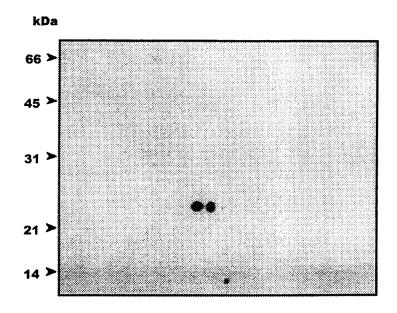


FIG. 2A

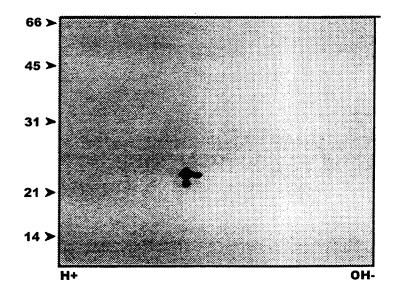
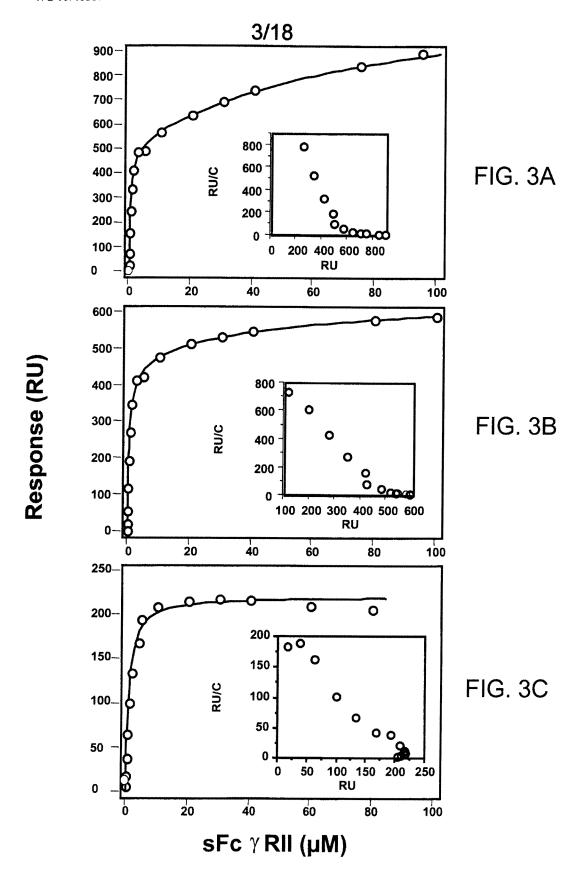


FIG. 2B



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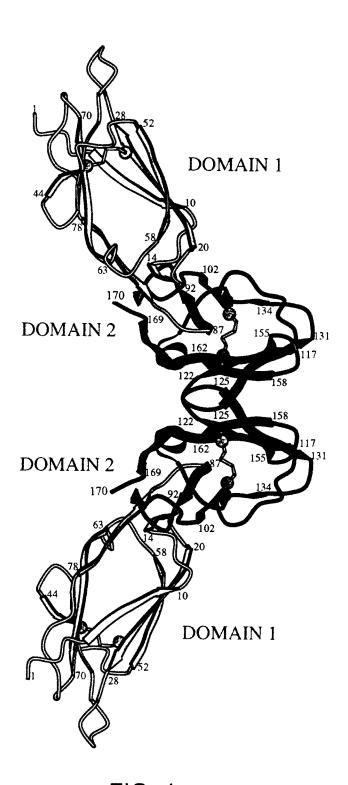


FIG. 4
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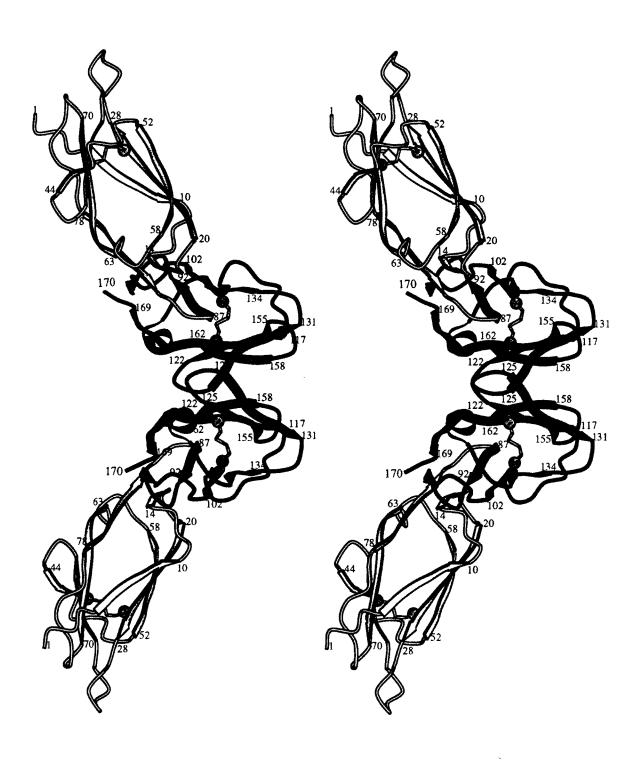


FIG. 6
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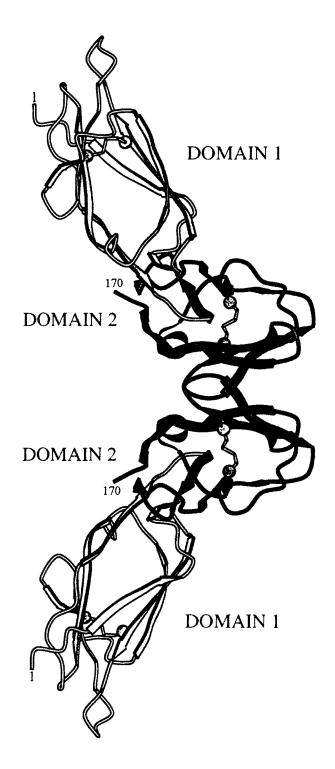


FIG. 7
SUBSTITUTE SHEET (RULE 26)

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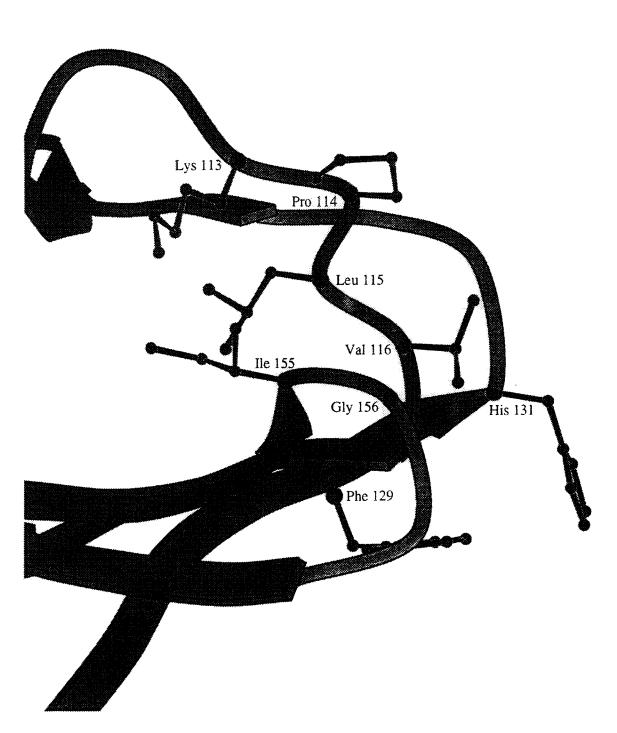


FIG. 8 SUBSTITUTE SHEET (RULE 26)

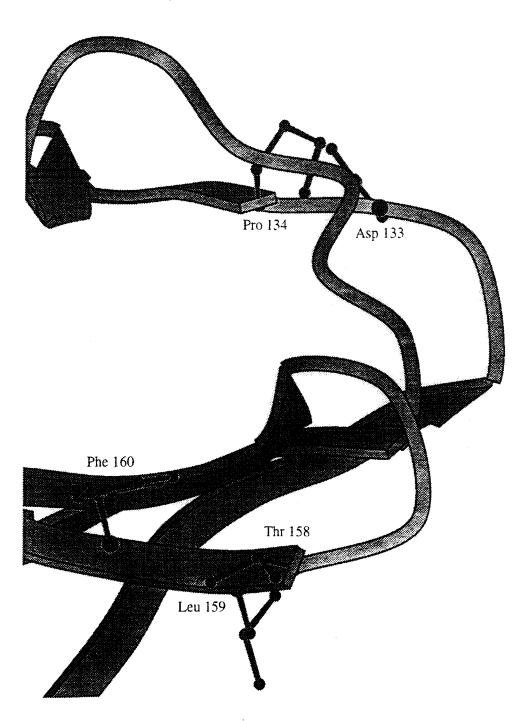


FIG. 9
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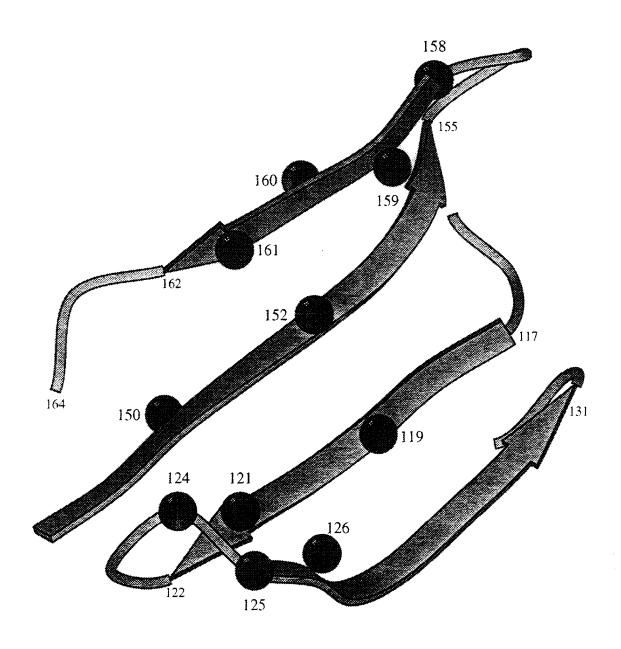


FIG. 10 SUBSTITUTE SHEET (RULE 26)

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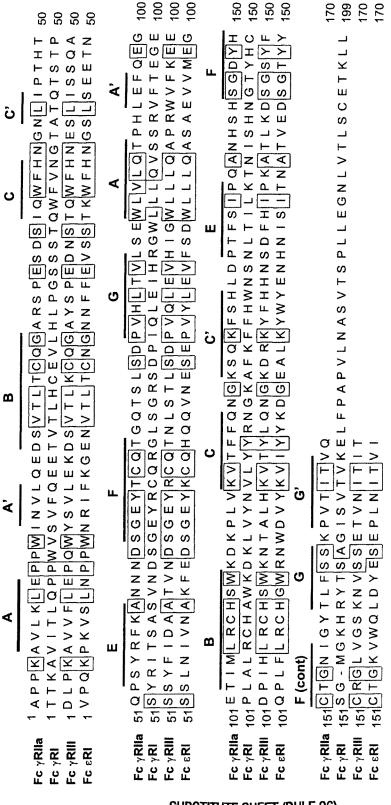


FIG. 11

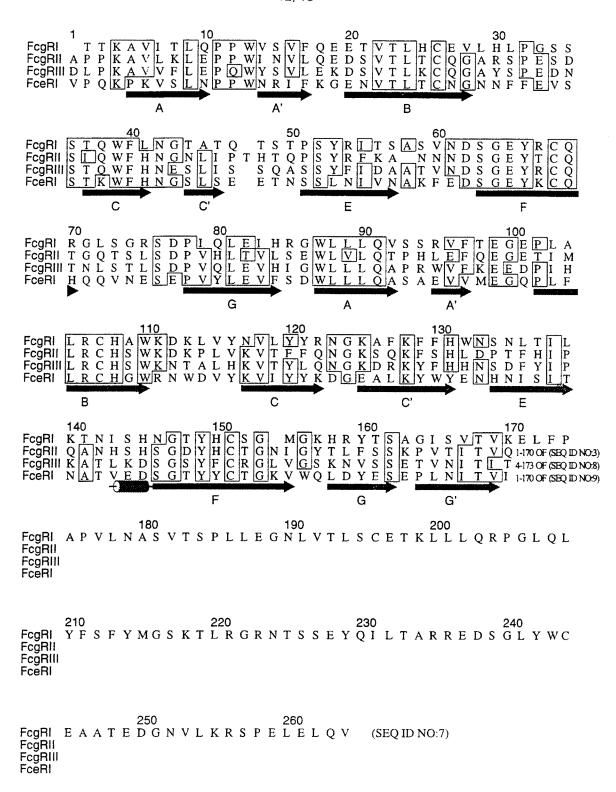


FIG. 12

SUBSTITUTE SHEET (RULE 26)

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Sequence FcgRIIa 1-171

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Sequence FceRI 1-172

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YKCQHQQVNESEPVYLEVFSDWLLLQASAEVVMEGQPLFLRCHGWRNWDVYKVIYYKDGEALKYW

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FIG. 13

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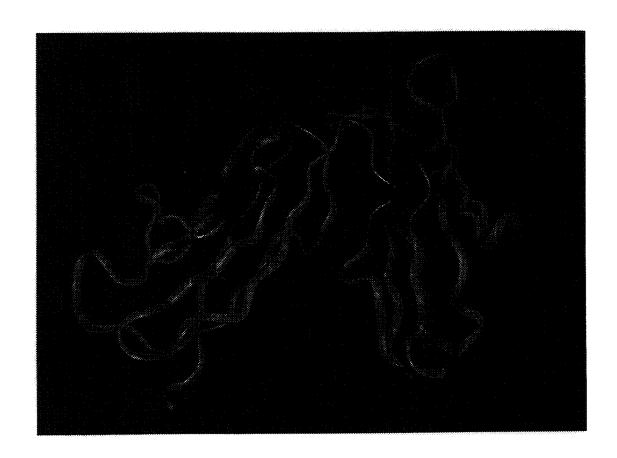


FIG. 14

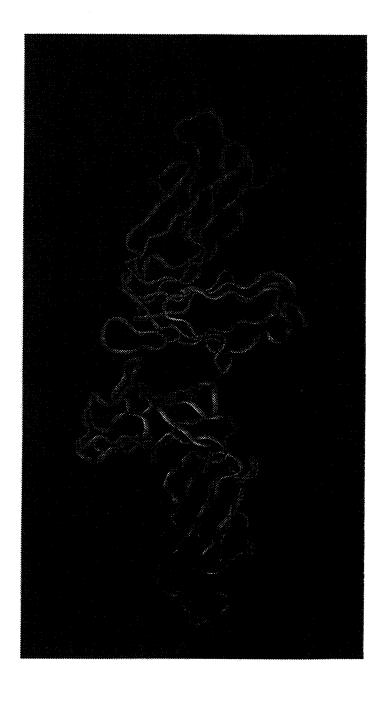


FIG. 15

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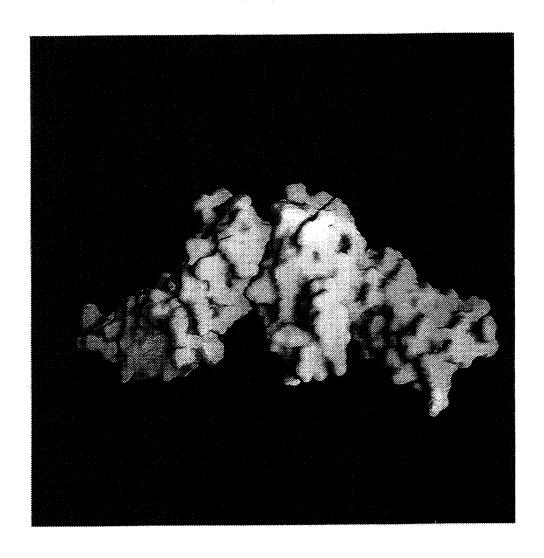


FIG. 16

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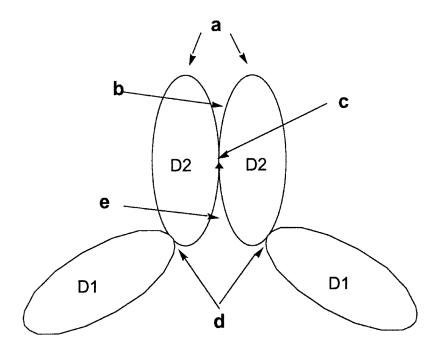


FIG. 17

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fcgr2a	THTQPSYRFK	-ANNNDSGEY	TCQTGQTSLS	${\tt DPVHLTVLFE}$	WLVLQTPHLE
fcgr3b	SQ-ASSYFID	AATVNDSGEY	RCQTNLSTLS	DPVQLEVHIG	WLLLQAPRWV
fcgr2a	FQEGETIMLR	${\tt CHSWKDKPLV}$	${\tt KVTFFQNGKS}$	QKFSHLDPTF	SIPQANHSHS
fcgr3b	FKEEDPIHLR	CHSWKNTALH	KVTYLQNGKD	RKYFHHNSDF	HIPKATLKDS
fcgr2a	GDYHCTGNIG	YTLFSSKPVT	ITV-QV	(.	SEQ ID NO:3)
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FIG. 18

SEQUENCE LISTING

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Cys	Glu	Thr 195	Lys	Leu	Leu	Lys	Gln 200	Arg	Pro	Gly	Leu	Gln 205	Leu	Tyr	Phe
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Leu Glu Val Phe Ser Asp Trp Leu Leu Leu Gln Ala Ser Ala Glu Val 85 90 95

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8

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Thr Cys Ser Ser Ala His Ile Pro Phe Asp Arg Phe Ser Leu Ala Lys 145 150 155 160

Glu Gly Glu Leu Ser Leu Pro Gln His Gln Ser Gly Glu His Pro Ala 165 170 175

Asn Phe Ser Leu Gly Pro Val Asp Leu Asn Val Ser Gly Ile Tyr Arg 180 185 190

Cys Tyr Gly Trp Tyr Asn Arg Ser Pro Tyr Leu Trp Ser Phe Pro Ser

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His Leu Thr Val Leu Ser Glu Trp Leu Val Leu Gln Thr Pro His Leu 85 90 95

Glu Phe Gln Glu Gly Glu Thr Ile Met Leu Arg Cys His Ser Trp Lys 100 105 110

Asp Lys Pro Leu Val Lys Val Thr Phe Phe Gln Asn Gly Lys Ser Gln 115 120 125

Lys Phe Ser His Leu Asp Pro Thr Phe Ser Ile Pro Gln Ala Asn His 135 Ser His Ser Gly Asp Tyr His Cys Thr Gly Asn Ile Gly Tyr Thr Leu 150 Phe Ser Ser Lys Pro Val Thr Ile Thr Val Gln 165 <210> 15 <211> 171 <212> PRT <213> Homo sapiens Ala Ala Pro Pro Lys Ala Val Leu Lys Leu Glu Pro Pro Trp Ile Asn 5 10 Val Leu Gln Glu Asp Ser Val Thr Leu Thr Cys Gln Gly Ala Arg Ser 25 Pro Glu Ser Asp Ser Ile Gln Trp Phe His Asn Gly Asn Leu Ile Pro 40 Thr His Thr Gln Pro Ser Tyr Arg Phe Lys Ala Asn Asn Asn Asp Ser 55 Gly Glu Tyr Thr Cys Gln Thr Gly Gln Thr Ser Leu Ser Asp Pro Val 65 His Leu Thr Val Leu Phe Glu Trp Leu Val Leu Gln Thr Pro His Leu 90 Glu Phe Gln Glu Gly Glu Thr Ile Met Leu Arg Cys His Ser Trp Lys Asp Lys Pro Leu Val Lys Val Thr Phe Phe Gln Asn Gly Lys Ser Gln 120 Lys Phe Ser His Leu Asp Pro Thr Phe Ser Ile Pro Gln Ala Asn His 130 135 140 Ser His Ser Gly Asp Tyr His Cys Thr Gly Asn Ile Gly Tyr Thr Leu 145 150

Phe Ser Ser Lys Pro Val Thr Ile Thr Val Gln 165 170

INTERNATIONAL SEARCH REPORT

International application No.

PCT/IB 99/00367

A.	CLASSIFICATION OF SUBJECT MATTER							
Int Cl ⁶ :	C07K 14/735, A61K 38/17, G06T 15/00, G06T 17/40							
According to International Patent Classification (IPC) or to both national classification and IPC								
В.	B. FIELDS SEARCHED							
Minimum documentation searched (classification system followed by classification symbols) IPC ⁶ , IPC ⁵ A61K, C07K								
Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched								
Electronic data base consulted during the international search (name of data base and, where practicable, search terms used) MEDLINE, FCR, CRYST, ELECTRON DENSITY MAP, THREE DIMENSIONAL STRUCTURE, X-RAY, CA, WPIDS DIFFRACTION DRUG DESIGN, COMPUTER STN: - SEQUENCE SEARCH USPTO TEXT & IMAGE DATABASE - PROTEIN, IMAGE, COMPUTER, RECEPTOR, 3-DIMENSIONAL								
C.	DOCUMENTS CONSIDERED TO BE RELEVAN	т						
Category*	Category* Citation of document, with indication, where appropriate, of the relevant passages							
X A	49, 55, 56, 75, 76							
X A	81							
X	Further documents are listed in the continuation of Box C	See patent family an	nex					
"A" document not come the interest of the inte	al categories of cited documents: "Interest defining the general state of the art which is ansidered to be of particular relevance application or patent but published on or after ernational filing date tent which may throw doubts on priority claim(s) ch is cited to establish the publication date of er citation or other special reason (as specified) tent referring to an oral disclosure, use, tion or other means ent published prior to the international filing ut later than the priority date claimed	priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art						
Date of the actu 30 June 1999	al completion of the international search	Date of mailing of the international search report 0 9 JUL 1999						
		Authorized officer K. G. ENGLAND Telephone No.: (02) 6283 2292						

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International application No.
PCT/IB 99/00367

tion). DOCUMENTS CONSIDERED TO BE RELEVANT	207
Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Padlan, E. A., Helm, B.A. BIOCHEMICAL SOCIETY TRANSACTIONS Vol 21 (1993) pp 963 - 967 See whole document	1-14, 16, 49
Burmeister, W.P.; Gastinel, L. N. et al NATURE V 372, pp 336 - 343 24 November 1994	49
Burmeister, W. P.; Huber, A.H. et al NATURE V 372, pp 379 - 383 24 November 1994	49
Weng, Z.; Gulukota, K. et al J. MOL. BIOL (1998) 282 pp 217 - 225	
	Citation of document, with indication, where appropriate, of the relevant passages Padlan, E. A., Helm, B.A. BIOCHEMICAL SOCIETY TRANSACTIONS Vol 21 (1993) pp 963 - 967 See whole document Burmeister, W.P.; Gastinel, L. N. et al NATURE V 372, pp 336 - 343 24 November 1994 Burmeister, W. P.; Huber, A.H. et al NATURE V 372, pp 379 - 383 24 November 1994